Evaluation of the Engineering Design Study Testing of the Batch Supercritical Water Oxidation Process to Treat NSCMP Neutralents and CAIS Materiel

Prepared for:

Non-Stockpile Chemical Materiel
Program Manager

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Stone & Webster, Inc.
A Shaw Group Company

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J.A. Bettinger
R. Weiler
Dr. J.M. Cardito

Approved By: _____
Stone & Webster Project Manager

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NSCMP Task Manager

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EXECUTIVE SUMMARY

This report evaluates the results of the Engineering Design Study Testing of the Batch Supercritical Water Oxidation (Batch-SCWO) process currently being developed by Sandia National Laboratories in Livermore, California (Sandia). Stone & Webster, Inc. conducted these tests on behalf of Non-Stockpile Chemical Material Program (NSCMP) (Edward F. Doyle III, Team Leader for Alternative Systems Demonstration and Evaluation Group) to evaluate the applicability of the process to the treatment of NSCMP neutralents. The Batch-SCWO process is developmental and all testing was conducted at the laboratory/bench scale. The test program was initiated at Sandia in February 2001 and culminated with a performance test that occurred over the period of June 1 – 7, 2001.

The Batch-SCWO process operates at conditions of pressure and temperature (4,000 psia and 600 ^{o}C) similar to the continuous SCWO processes, but on a single batch basis. The material is introduced into the process vessel with an appropriate oxidant; heated to operating temperature; and held for the reaction residence time. The process vessel and contents are then cooled, depressurized (through an appropriate filter) and sampled to ensure the efficacy of the treatment. The residuals may then be disposed of, or the process repeated as necessary. The batch mode of operation, specifically the final cooling step, eliminates the difficulties associated with salts generated within the system during treatment that are observed in continuous flow systems.

The principal objectives of the testing were to assess the Batch-SCWO process' applicability to processing NSCMP liquid neutralents and Chemical Agent Identification Set (CAIS) materiels. Two neutralent simulants and a simulated CAIS vial were tested. The process was evaluated based on six test objectives:

1. Demonstrate the applicability of the Batch SCWO process to treating liquid NSCMP neutralents by processing simulants.
2. Demonstrate the applicability of the Batch SCWO process to treating CAIS by processing simulated CAIS vials.
3. Determine the fate of relevant heteroatoms contained in the feed material during operation of the Batch SCWO system.
4. Provide basic engineering data to evaluate the practicality for implementation in the NSCMP.
5. Quantify and document key operating and engineering design parameters to support the conceptual design package.
6. Develop a plan including concept design for the next phase of testing.

Data and observations from the tests were evaluated in accordance with established criteria. Test conclusions based on these criteria are summarized below.

- Nine out of ten tests at 600 ^{o}C demonstrated a destruction efficiency, based on TOC, of greater than 99.99 % for simulated GB and H neutralents. One test that did not make this target achieved a destruction efficiency of 99.988%.
- All tests at 600 ^{o}C demonstrated the ability of Batch-SCWO to process simulated GB and H neutralents and achieve a residual liquid TOC of less than 5 ppm. In 8 of the ten tests, the TOC was below the detection limit of 1.0 ppm.
- The Batch-SCWO process demonstrated a repeated and consistent ability to burst simulated K952 CAIS vials in the enclosed process during heatup.
- The liquid residuals from the process contained various concentrations of metals attributed to corrosion of the reactor vessel indicating that materials of construction and corrosion management need to be addressed through additional study in subsequent phases.
- The vapor residual from the tests at 600 ^{o}C, contained trace amounts (tens of parts-per-billion) of several volatile organic compounds, but none were at a level to pose a problem with permitting a system.
- The bench-scale system had several equipment-related problems (valve leakage and cold spots in instrumentation), that can be eliminated in subsequent designs.
- Based on the test results, preliminary concepts were developed for a two-step scale up of the process. The pilot-scale system is a 5 to 6 gallon vessel to demonstrate the ability to process simulated munitions as well as simulated CAIS and CAIS materiel. The full-scale system is a 106-gallon vessel that could process whole munitions and intact CAIS.
- Stress analyses of the conceptual processing vessels for the scale-up steps were completed to evaluate the Batch-SCWO operating concept's practicality in fabrication and operation. The process, as conceptualized, did not exceed allowable stresses and is feasible for the intended use.

Based on these conclusions, the following is recommended:

- It is recommended that the Batch-SCWO process development proceed to the next level (Phase 2), which is the fabrication and testing of a 5 to 6 gallon pilot-scale unit capable of processing:
  - Simulated munitions
  - Simulated CAIS and actual CAIS components.
- A rigorous material of construction and corrosion management testing and evaluation program should be initiated to identify appropriate materials of construction and provide a quantitative indication of the reliability of the materials for pilot and full-scale operation.

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List of Acronyms and Abbreviations

ACRONYMS & ABBREVIATIONS	DEFINITIONS
ACWAP	Assembled Chemical Weapons Assessment Program
ATAP	Alternative Technologies and Approaches Program
ASME	American Society of Mechanical Engineers
BHO	Batch Hydrothermal Oxidation
CAIS	Chemical Agent Identification Set
CDP	Chemical Demilitarization Program
CG	Chemical agent, Phosgene
CK	Chemical agent, Cyanogen Chloride
CN	Chemical agent, Chloracetophenone
CWC	Chemical Warfare Convention
CWM	Chemical Warfare Materiel
DCE	1,2-dichloroethane
DM	Chemical agent, Adamsite
DMMP	Dimethyl methylphosphonate
DMSO	Dimethyl sulfoxide
ECBC	Edgewood Chemical and Biological Command
EDS	Explosive Destruction System
EPA	Environmental Protection Agency
GA	Chemical agent, Tabun
GB	Chemical agent, Nerve agent, Sarin
GC	Gas Chromatography
H	Chemical agent, Mustard
HD	Chemical agent, Sulfur Mustard (distilled)
HETM	N-(2-hydroxyethyl)-thiomorpholine
HN	Chemical agent, Nitrogen Mustard
HTO	Hydrothermal Oxidation
L	Chemical agent, Lewisite
MAWP	Maximum Allowable Working Pressure
MEA	Monoethanolamine
MMD	Munitions Management Device
MS	Mass Spectroscopy
NMR	Nuclear Magnetic Resonance
NO_x	Nitrogen Oxides
NSCM	Non-Stockpile Chemical Materiel
NSCMP	Non-Stockpile Chemical Materiel Program
ORP	Overarching Research Plan
PC	Personal Computer
PDHID	Pulsed Discharge Helium Ionization Detector
PMCD	Program Manager for Chemical Demilitarization
ppb	Parts per billion

ACRONYMS & ABBREVIATIONS	DEFINITIONS
ppm	Parts per million
PS	Chemical agent, Chloropicrin
psi	Pound per Square Inch
RCRA	Resource Conservation and Recovery Act
SCWO	Supercritical Water Oxidation
SwRI	Southwest Research Institute
TAP	Technical Analysis Procedure
TCD	Thermal Conductivity Detector
TOC	Total Organic Carbon
VOC	Volatile Organic Compound
Wt	Weight

Evaluation of the Engineering Design Study Testing of the Batch Supercritical Water Oxidation Process to Treat NSCMP Neutralents and CAIS Materiel

1. Introduction

This report evaluates the results of the Engineering Design Study Testing of the Batch Supercritical Water Oxidation (Batch-SCWO) process currently being developed by Sandia National Laboratories in Livermore, California (Sandia). Stone & Webster managed these tests to evaluate the process' applicability to the treatment of Non-Stockpile Chemical Materiel Program (NSCMP) feeds. The Batch-SCWO process is developmental and all testing was conducted at the laboratory/bench scale.

Sandia conducted the testing under a "Research for Others" grant that was administered directly by the NSCMP. Technical management was provided for NSCMP by Stone & Webster under their Program and Integration Support Contract. Stone & Webster also subcontracted Southwest Research Institute (SwRI) for analytical services during the performance test.

This section discusses the objectives of the Engineering Design Study Tests and the Evaluation Criteria that Stone & Webster developed to assess the Batch-SCWO process performance. Section 2 of this report provides background information on the technology as well as the rationale for selecting Batch-SCWO for testing. Section 3 describes the bench-scale unit that was tested. Section 4 describes the testing approach, procedures and all of the test runs completed. The results of the tests are presented in Sections 5 and 6. Section 5 is a discussion of the testing that was conducted on NSCMP neutralent wastes. Section 6 presents the testing of Chemical Agent Identification Sets (CAIS). Section 7 contains a discussion of the Batch-SCWO process' applicability to the NSCMP, including concepts for full-scale applications. Sections 8 and 9 include the test conclusions and recommendations for further action.

1.1 Objectives

The overall objective was to perform testing to determine the applicability of the Batch Supercritical Water Oxidation (Batch-SCWO) Process system to treat NSCMP neutralents and CAIS materiels in a mobile system. To support evaluation of this objective, Stone & Webster developed a series of test objectives and criteria that would allow unambiguous determination as to whether the specific test objectives have been met. These test objectives were the basis for the formulation of the test plan and included:

1) Demonstrate the applicability of the Batch SCWO to treating liquid NSCMP neutralents by processing simulants.
2) Demonstrate the applicability of the Batch SCWO to treating CAIS by processing simulated CAIS vial.
3) Determine the fate of relevant heteroatoms contained in the feed material during operation of the Batch SCWO system.

4) Provide basic engineering data to evaluate the practicality for implementation in the NSCMP.
5) Quantify and document key operating and engineering design parameters to support the conceptual design package.
6) Develop a plan including concept design for the next phase of testing.

1.1.1 Treat NSCMP Neutralent Material

The ability of the Batch-SCWO process to adequately treat neutralent material was evaluated to determine the applicability of the system to use as a treatment system in conjunction with an established CWM processing module. Current NSCMP potential processing options include removing the agent materiel from its carrier and neutralizing it with a mono-ethanolamine (MEA) solution. The neutralent, while "agent-free," still contains a significant amount of organic byproducts including some Schedule 2 compounds. In all cases, the neutralent requires additional treatment prior to discharge. Batch-SCWO has the potential to be an effective secondary treatment of this neutralent.

1.1.2 Treat CAIS Materiel

The NSCMP inventory contains significant numbers of Chemical Agent Identification Sets (CAIS). These sets consist of chemical agents placed in glass ampoules, vials and bottles, then packaged in metal shipping containers or wooden boxes. Various types of CAIS were manufactured and widely distributed to military and civilians groups, and are periodically recovered at a variety of locations throughout the United States.

CAIS materiels present a unique disposal problem. While there are generally four types of containers (all 2 to 4 ounce glass bottles or vials), there are 22 different variations of contents including neat agent, agent deposited on charcoal and industrial chemicals. Currently recovered CAIS materiels are evaluated and segregated for neutralization (chemical agent) or repackaging for disposal as industrial waste (industrial chemical). There are four different processes for neutralizing CAIS materiels. Batch-SCWO has the potential to be a "universal CAIS processing system" in that a system could potentially be developed that is capable of processing all types of CAIS with one process.

Critical to the ability to process the CAIS materiel is demonstration of the ability to access the contents of the container. Testing was conducted to determine if Batch-SCWO processing could reliably access the contents of simulated CAIS vials.

1.1.3 Fate of Heteroatoms and Material Balance Closure

One of the key criteria that is being used to evaluate all processing systems for NSCMP applications is their destruction efficiency. Accurate determination of this is based on a system material balance. That is, the feed is analyzed to determine the initial amount of a compound. The residual is analyzed for the same material and the difference in mass is the amount destroyed. This evaluation technique assumes that the laboratory analyses are accurate and all material is recovered. In the bench/laboratory-scale of testing that was used for the Batch-

SCWO process, small inaccuracies in analyses or recovery can have significant impacts on the destruction calculation. A material balance is an effective way to evaluate the accuracy of the destruction calculations.

One reported advantage of the Batch-SCWO process is that the bulk of the heteroatoms (Chlorine, Sulfur and Fluorine) remain in the liquid phase, thereby eliminating or reducing the need for scrubbing the gaseous discharge. The process residuals will be analyzed to evaluate the disposition of relevant heteroatoms. As discussed above, closure of the materials balance will validate the results.

1.1.4 Evaluate the Practicality for NSCMP

The Batch-SCWO process is being evaluated for use by the NSCMP as a mobile unit to process neutralent or potentially CWM. In order for the system to be of use there must be a certain level of practicality in the configuration and operation of the process. For example, there are size and weight limitations associated with transport. In addition, the system must be robust in both the process and equipment and be able to sustain a reasonable throughput, availability and reliability.

It is recognized that this is a vague objective, however the goal is to obtain sufficient data at the bench-scale to develop a process concept for an implementable system that can be evaluated for practicality in operation.

1.1.5 Develop Full-scale Processing Concept

The bench-scale testing will be the basis for developing a full-scale processing concept. Several possible operating scenarios and potential applications exist for the Batch-SCWO process. The system can be used to process MEA-based neutralent that is generated by processing CWM either at a fixed or mobile facility.

An alternative concept is to process individual CWM in the Batch-SCWO vessel. For example, CAIS vials may be loaded into the vessel with sufficient oxidant and the unit sealed. As the vessel heats up the CAIS vial would burst and the contents would be oxidized. Once the oxidation was complete, the vessel could be cooled and destruction verified through sampling and the contents removed. On a larger scale, individual munitions could be placed into the vessel, which is sealed and the munition accessed through a controlled detonation initiated by shape charges (in a manner similar to the existing Explosive Destruction System). Once the munition is detonated, the system is heated to SCWO conditions and the agent is destroyed. The system would be cooled, sampled and contents discharged once destruction is verified.

An objective of the bench-scale testing is to develop a basic understanding of the process, including limitations, in order to develop a processing concept for a full-scale system. At this time, two full-scale concepts are anticipated. The first would be a unit capable of processing individual CAIS materiels and a second, larger unit that could process complete live munitions. The larger unit would be based on processing a 4.2-inch mortar as this represents the most numerous item in the current non-stockpile inventory.

1.1.6 Develop Plan for Next Phase of Testing

Recognizing that this phase of testing was at the bench-scale, the results would simply indicate the validity of the processing concept. Even in the best case, favorable results would not provide sufficient design data to support full-scale system design. However, based on the favorable results, a plan could be developed for the next phase of testing to both evaluate the concept at a prototypical scale, and develop sufficient data to support full-scale system design.

1.2 Evaluation Criteria

Associated with the six test objectives are specific criteria that were used to evaluate the effectiveness of the testing. The evaluation criteria and associated objectives are discussed below.

1.2.1 Treat NSCMP Neutralent Material

The effectiveness of the Batch-SCWO process to treat neutralent material was evaluated based on the following criteria:

- Stable operation with all systems controlled and no system function overridden for the duration of the tests.
- Target destruction efficiency of at least 99.99% with less than 10 ppm TOC in liquid effluent.
- Liquid effluents meet limits for disposal from Federal Wastewater Treatment Facility
- Solid residuals can be disposed of at RCRA facility
- Gaseous effluents are permittable
- Identification of additional treatment steps

1.2.2 Treat CAIS Materiel

Critical to effective treatment of the CAIS materiel is the ability of the Batch-SCWO process to access the CAIS vial or bottle. While it was originally intended to evaluate both accessing the vial and destroying the contents, the size of the bench-scale processing vessels limited the ability to evaluate destruction. Therefore the testing focused on accessing the vial contents. The effectiveness of the Batch-SCWO process to treat CAIS materiel was evaluated based on the following criteria:

- Ability to access the vial contents
- Stable operation with all systems controlled and no system function overridden for the duration of the tests.

1.2.3 Fate of Heteroatoms and Material Balance Closure

This objective applied to the neutralent processing only since that was the only testing that was directed towards quantifying the destruction of organic constituents. The following criteria were applied:

- Material balance closure for Fluorine, Chlorine, and Sulfur.
- Overall material balance

1.2.4 Evaluate the Practicality for NSCMP

A subjective evaluation of the overall Batch-SCWO process practicality for use in the NSCMP overall program and mission was conducted based on the data generated by the bench-scale testing and the following criteria:

- Projected system size for treating CAIS
- Process operating characteristics
- System throughput
- Equipment operating characteristics
- System safety including engineered safeguards
- Reliability, availability and maintainability
- Fabrication and operational costs
- Permitability

1.2.5 Develop Full-scale Processing Concept

The following items were evaluated to develop an understanding of the process to support the processing concept:

- Key operating parameters
- Design Margins
- Critical scale-up parameters,
- Core technology scale-up parameters, and
- Solids handling.

1.2.6 Develop Plan for Next Phase of Testing

The bench-scale testing was a first step in process development to understand the process and its limitations. Based on the test results, a plan for the next phase of testing was developed and the resulting plan evaluated against the following criteria:

- Plan objectives consistent with NSCMP needs
- Equipment/process of a size to confirm/validate critical process and component design/scale-up factors
- Reasonableness/realism
- Design/concept safety
- System use beyond the test program

2. Background

2.1 Technology Evaluation and Development for NSCMP

The U.S. Army Program Manager for Chemical Demilitarization (PMCD) established the NSCMP with the mission to provide centralized management and direction to the Department of Defense for the disposal of non-stockpile chemical materiel in a safe, environmentally sound and cost effective manner. The NSCMP includes five categories of chemical warfare materiel (CWM): binary chemical weapons; former production facilities; miscellaneous CWM; recovered chemical weapons; and buried CWM. Substantial differences exist between CWM in the Stockpile and Non-Stockpile programs. Whereas the stockpiled CWM is present in larger quantities, non-stockpile CWM encompasses a greater variety of materiel with far more physical configurations and agent-fill types. The variety, locations and deteriorated physical condition of non-stockpile CWM pose unique requirements for treatment systems.

To support accomplishment of its mission, the NSCMP developed an Overarching Research Plan[1] (ORP) which establishes the goals, requirements, and approaches for evaluating and developing technologies for the safe and efficient disposal of non-stockpile CWM. The ORP identifies systems that NSCMP has and is continuing to develop to meet its mission goals. The ORP also identifies additional needs and associated schedule to support accomplishment of these goals. The ORP identified Near-Term, Intermediate-Term and Long-Term applications for technologies to treat the broad range of NSCMP wastes.

To meet these needs, NSCMP has identified several additional systems for application to non-stockpile CWM based on the results of technology evaluations and demonstration testing performed as part of the PMCD Alternative Technologies and Approaches Program (ATAP) and the Assembled Chemical Weapons Assessment Program (ACWAP).

In May 2000 NSCMP identified the Batch Hydrothermal Oxidation Process (BHO) process under development by Sandia National Laboratories (Sandia) as one of the promising long-term CWM treatment systems. The BHO process was developed and patented by Sandia (U.S. Patent number 6,030,587) based on an internally heated vessel with cooled sides that establishes an internal circulation with a limited reaction zone in the center that is at supercritical conditions, while the balance of the vessel is maintained at subcritical conditions. Key to the patent claims is that the vessel is heated by an element that projects into the interior of the vessel, and maintaining the walls cool to establish the internal circulation.

At the May meeting, Sandia presented past work on Batch-SCWO and BHO. BHO was presented as a method of reducing the volume of a Batch-SCWO reactor. Sandia proposed a development program to NSCMP for the BHO process to be used in conjunction with (or a manner similar to) the Explosive Destruction System (EDS) that was also under development by Sandia. It is significant to note that the proposed BHO system would operate in a mixed sub-and supercritical regime by establishing the internal circulation as described in the Sandia patent.

NSCMP charged Stone & Webster with conducting an evaluation of the Sandia BHO process. Stone & Webster concluded in October 2000, that scaling up the BHO process to EDS size and

overcoming the mechanical challenge of fitting internals (heaters and baffles to establish circulation) that would withstand detonation as well as processing conditions would be a major development effort. Stone & Webster recommended that a more practical alternative would be to develop a batch reactor that would operate at supercritical conditions, without the internals needed to create the two phases for true BHO operation. Based on that recommendation, the Batch Supercritical Water Oxidation (Batch-SCWO) processing concept was set.

2.2 Supercritical Water Oxidation

In February 2001, Stone & Webster and NSCMP (Edward F. Doyle III, Team Leader initiated a test program for Alternative Systems Demonstration and Evaluation Group) with Sandia to evaluate the Batch-SCWO process for NSCMP feeds. Targeted materials for this testing included surrogates of chemical agent neutralents, GB and H, as well as simulated CAIS vials.

Supercritical Water Oxidation (SCWO) is an aqueous oxidation process. It is similar to subcritical (or wet) oxidation processes in that oxidation of organic substances occurs in the presence of water at moderate temperatures. The major difference is that while subcritical systems are operated to maintain water in the liquid state and are called 'wet,' supercritical systems are operated above the critical point of water. Within the reaction zone, the water is not present as a conventional vapor (steam) or liquid. It exists as a supercritical fluid phase that is a hybrid with properties of both liquid and vapor. The supercritical fluid has unique solubility properties in that organic materials and gases are completely miscible, while inorganic materials are only slightly soluble. These properties remove the mass transfer limitations, and associated lower destruction efficiencies, of subcritical (wet) systems. This enhanced mass transfer combined with a moderate temperature of operation (374 - 600°C) results in a system capable of virtually complete destruction (99.99+%) of organic materials, while providing a means of separating and concentrating inorganic compounds.

A significant advantage of SCWO is that there are minimal air pollution problems compared with conventional incineration. The oxidation occurs in water, and acid gas formers (anions of S, P, and Cl) are soluble and exit the process as solutions, or in the case of nitrogen, as inert gases. NO_X is routinely less than 1 mg/m^3 in the gaseous effluent of any existing test unit. A significant advantage is that the main effluent streams are liquid and can be contained and tested prior to discharge.

Supercritical water oxidation systems have a solid history of bench scale testing, dating back to the early 1980's and have been shown to be capable of complete destruction of a variety of organic compounds. To date thousands of materials have been oxidized with bench and continuous units. However, previous demonstrations of this technology applied to continuous flow concepts have experienced limited success.

In the reaction zone, the organic material is oxidized at 600°C. Metals tend to precipitate as their oxides, while inorganic anions of Cl, S, and P form their respective acids. In the event these materials are present in quantities sufficient to effect corrosion through lowering pH, they are neutralized by the addition of NaOH. Experience has shown that reactor effluent pH should be maintained above 2 to minimize intergranular stress corrosion that could result in failures of high-nickel alloy pressure components. The anions present are neutralized to their corresponding salt form, which is insoluble in the supercritical fluid.

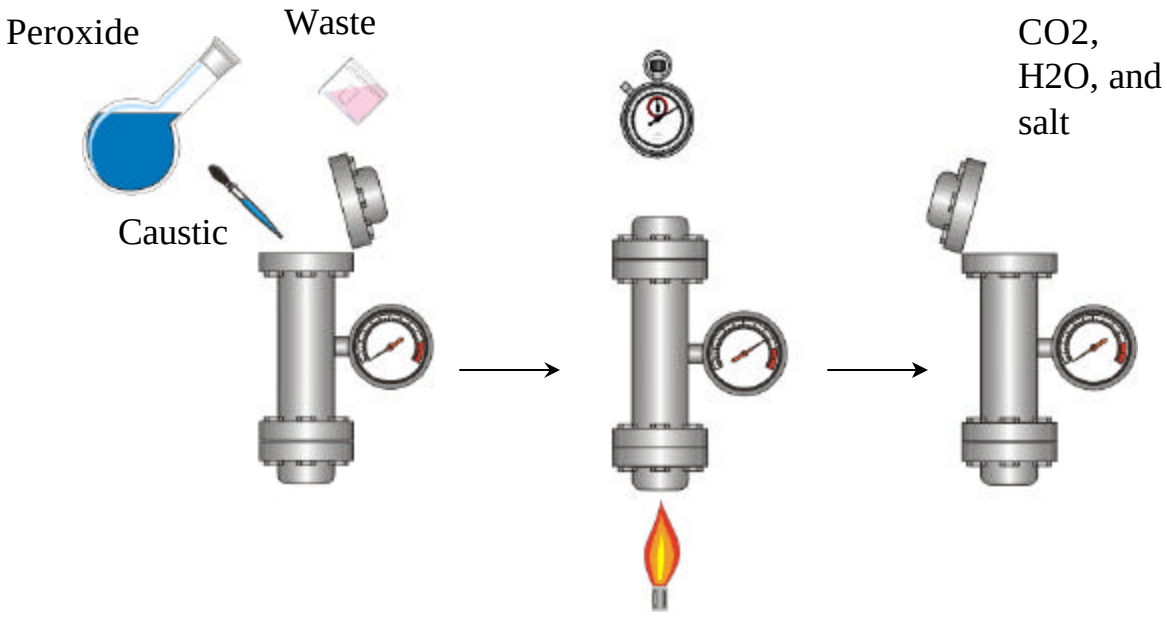
The major hurdle for the development of continuous flow processes is handling inorganic solids that are present or generated during processing. In the mid-1980's it was observed that when processing

a chlorinated waste that required neutralization, the resulting sodium salts plugged the reactor (sodium hydroxide was used as a neutralizing agent). Subsequent investigations showed that any feedstock that contains moderate amounts of halogens or acid precursors (Cl, S, P) must be neutralized to limit the corrosion of high-nickel alloys used in fabrication. An alternative to neutralization is to utilize a more corrosion resistant material. However in most cases the only corrosion resistant materials tend to be exotic and their associated costs and difficulties associated with fabrication techniques have limited their application.

To date the most effective neutralization technique has been in-situ through the addition of NaOH or $Ca(OH)_2$. However, while the neutralization is effective in minimizing corrosion, the resulting salts formed (NaCl, Na_2SO_4) are virtually insoluble in the supercritical fluid, and "sticky," depositing on the walls of the reactor or piping and eventually plugging the system. It has been observed that even when these sticky salts (NaCl, Na_2SO_4, and Na_2CO_3) are introduced into the reactor in their dissolved form (not generated in-situ), they are still sticky.

Although it is most often considered as a continuous flow process, SCWO can be used in a batch process (Batch-SCWO), see Figure 2-1. A batch reactor, which is conceptually like a pressure cooker, is mechanically and operationally much simpler, but is limited to smaller effluent streams. The reactants are loaded in the reactor at ambient pressure and temperature and then the reactor heated. The operating pressure is self-generated as the vessel is heated. A batch process is a logical choice for non-stockpile chemical materiel because of the inherent batch nature of individual munitions and because of the need for a small transportable system. Organic molecules are converted to the most benign products possible so problems with transporting and disposing of a hazardous waste stream are eliminated. The reaction takes place in a closed system so all products are contained and can be analyzed before the vessel is opened.

Figure 2-1 Batch-SCWO Processing Concept



3. System Description

The Engineering Design Study testing of the Batch-SCWO process to treat NSCMP neutralents and CAIS materiel was conducted at Sandia National Laboratories (Sandia) at their facilities in Livermore, California using bench-scale apparatus that was commercially procured and assembled by Sandia.

This section discusses the initial physical configuration of the test apparatus. During the testing, the system configuration evolved as experiments were conducted and limitations identified with the process and equipment. Specifically, during testing it was identified that material was collecting in the external tubing and instrumentation. Several modifications to the system were made to mitigate this phenomenon. While these problems provided valuable design information for the subsequent system design, they were basically external to the fundamental Batch-SCWO processing system and are discussed in Section 5 – Test Results and Discussion.

The Batch-SCWO reactor vessels for this testing were ASME-rated commercially procured items from Grayloc™ (see Figure 3-1). The reactors are made from Inconel 625™ and are rated at 7,425 psig maximum allowable working pressure (MAWP) at testing temperatures. They have an internal volume of 325 cc and are heated by two 465-Watt external band heaters. Figure 3-2 shows two vessels, one open, and the other closed and mounted in the test station. The test station, shown in Figure 3-3 and schematically in Figure 3-4, allows independent testing of up to four vessels simultaneously. The vessels use Grayloc™ metal gaskets to seal between the vessel and lid. A valve for filling and venting, a rupture disk for pressure safety, a pressure transducer and two thermocouples are connected to ports in the lid. Inconel 600™ sheathed thermocouples (1/16”) extend directly into the fluid. HIP™ clinch fittings secure the thermocouples in the lid and provide a pressure seal.

Temperatures are maintained with feedback temperature controllers using the thermocouples inside the reactor vessels. The controllers have a high-temperature shut-off for over-temperature protection. The reactors are also protected against over-pressure by burst disks. Temperature and pressure are monitored continuously throughout the operation and recorded on a 966 Odyssey™ data acquisition system. One thermocouple is located near the bottom in the vessel and another near the top. The lower thermocouple controls the vessel temperature. A third thermocouple measures the external wall temperature.

The unheated hardware is made from high pressure, 304 and 316 Stainless Steel and includes most tubing, transducers, and fittings. The tubing connecting the reactor to the pressure transducer and rupture disk is made of Hastalloy C™. A fill valve is used for both adding reagents, if necessary, and collecting or releasing product gases. Cooling of the reactors is done by forced convection of room air with four 110V electric fans.

The Batch-SCWO process layout is shown in Figure 3-4. Four reactors are placed inside insulated wells on a cart and can be operated simultaneously. Lex-guard shields are mounted on three sides of the cart for operator protection. The fourth side is backed against a fume hood. All gas vent lines are tied into a common tubing manifold that delivers the gases into the fumed hood.

Figure 3-1 Graylocô Reactor

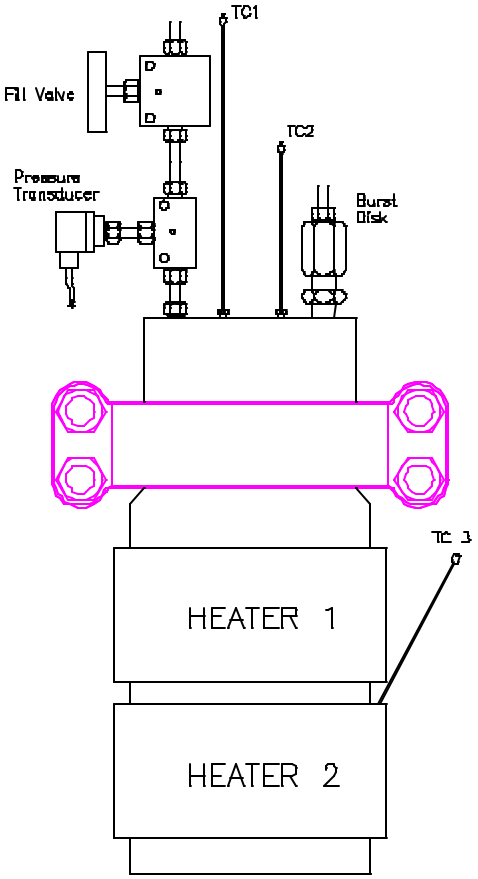


Figure 3-2 Test Reactors

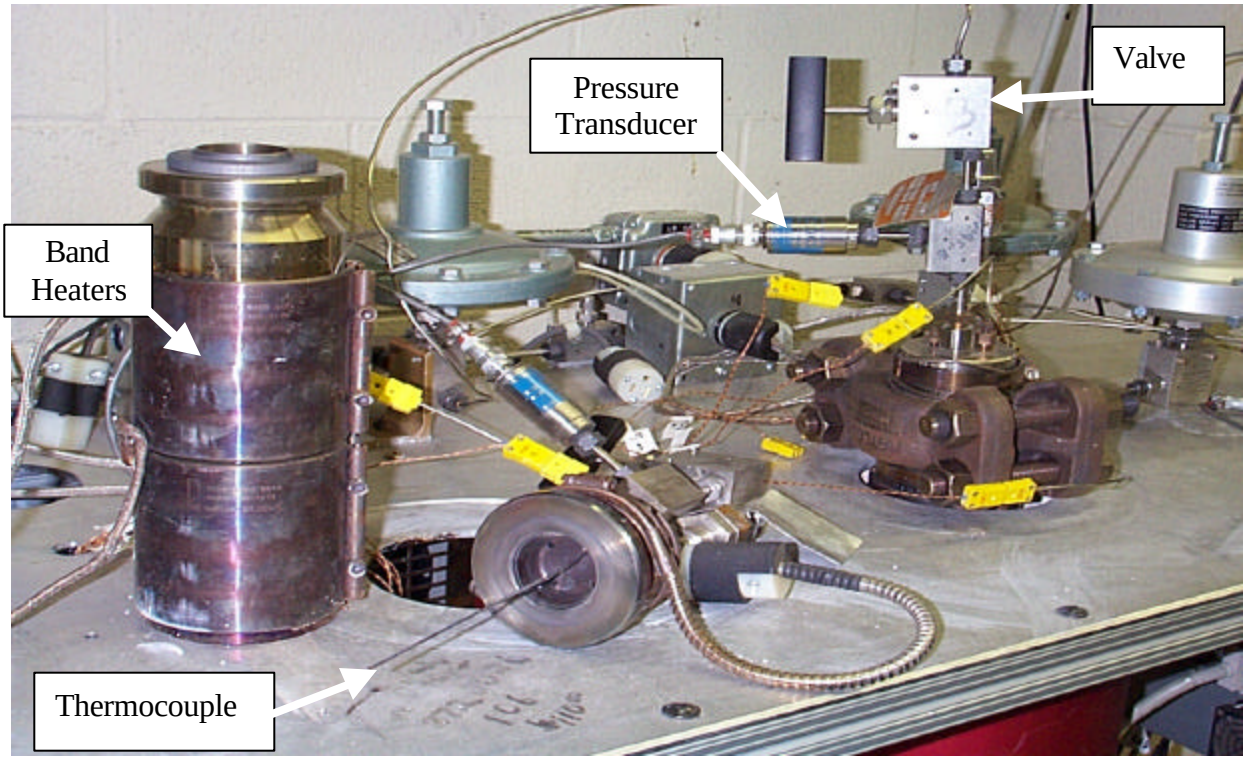


Figure 3-3 Test Station with Four Reactors

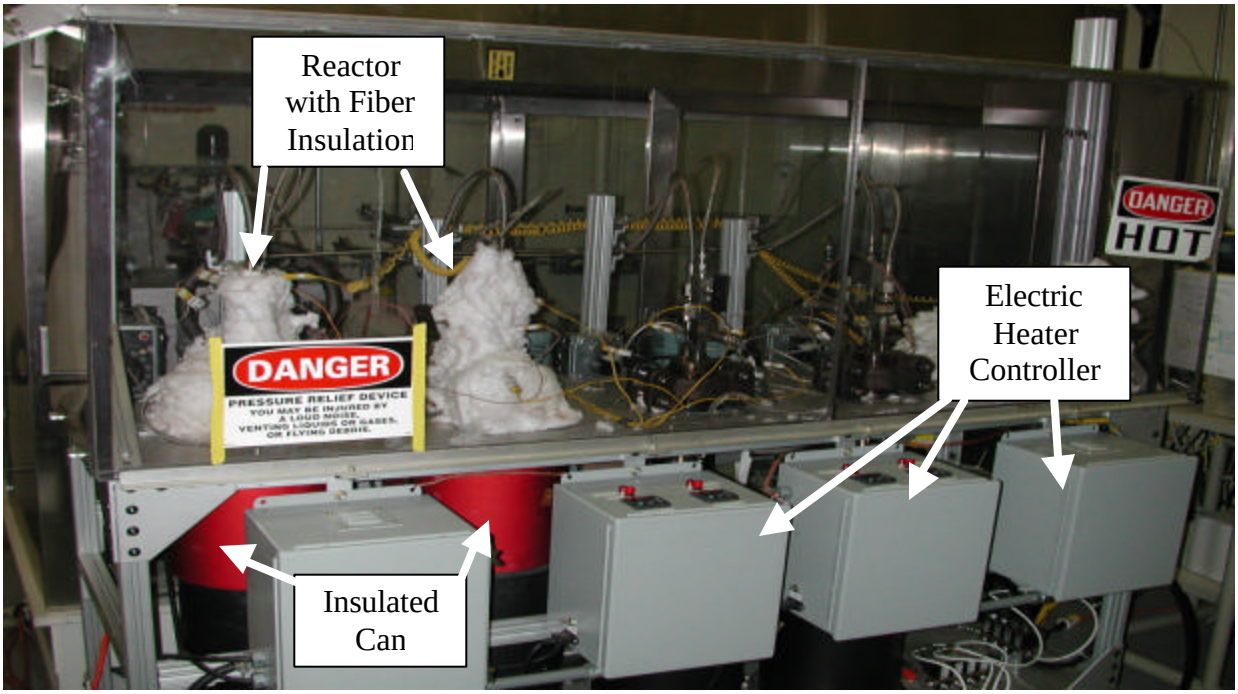
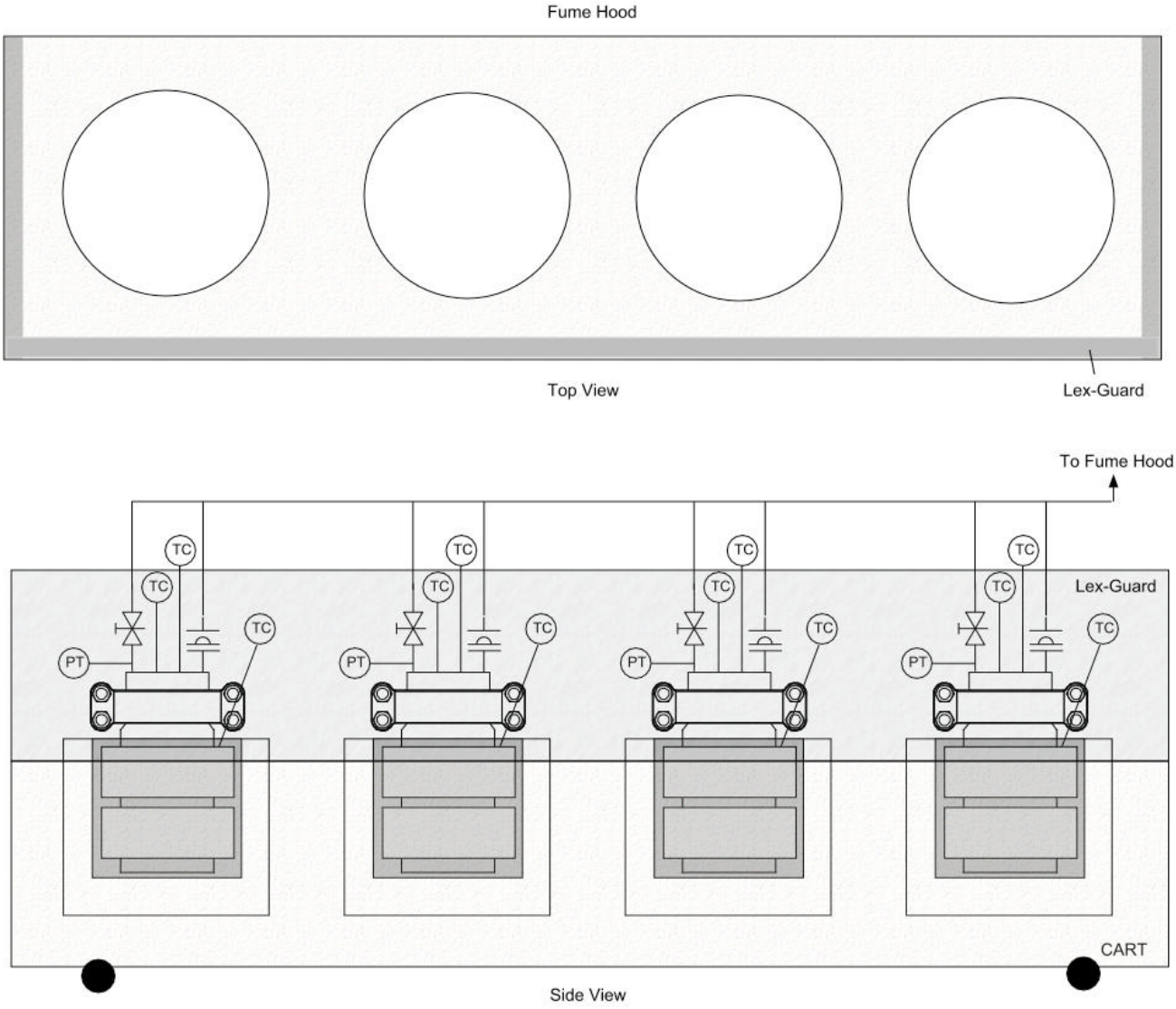


Figure 3-4 Batch-SCWO Reactor Set-up



4. Test Approach

This section provides a discussion of the workup and performance testing that was conducted at Sandia over the period of April through June 2000. Included are the original test matrix, feeds tested, and the specific procedures that were used for the tests. The results of testing are discussed in Sections 5 and 6 for the neutralent and CAIS simulants, respectively.

4.1 Test Matrix

The testing was originally structured to be completed in two series of testing campaigns. The system would be fabricated and a series of workup testing were to be conducted to shakedown the equipment and optimize the process and identify the operating conditions. Following the workup testing, a series of performance tests would be conducted with each feed material to validate the process. The performance tests were to be witnessed by Stone & Webster and all residuals collected for analysis by an independent laboratory (in this case SwRI).

4.1.1 Workup Testing

Initially the test plan was directed towards a series of workup tests to determine the operating procedures and conditions to achieve the targeted 10 ppm TOC in the residual liquid. The intent was to conduct parametric tests evaluating the influence of the following:

- Residence time (hold time at reaction temperature)
- Temperature
- Excess Oxidant
- Caustic Concentration

The workup testing was conducted from April 10 through May 30, 2001 to evaluate and develop an understanding of the influence of these reaction parameters in order to identify a set of "universal operating conditions" at which any of the potential feeds would achieve the destruction standards. A "universal operating conditions" approach was chosen to simplify operations later in the program by having one set of operating conditions that could be applied to any feedstock. Once the "universal operating conditions" were established in the workup runs, a series of performance tests were conducted and the residuals collected for analysis by an independent laboratory (SwRI).

However once the testing began, it was observed that there was a significant test-to-test variation in the residual TOC and the system was failing to meet the effluent criteria of 10 ppm TOC. This inconsistency was observed even in tests where the reactor contents were held at 600 ^{o}C for two hours, conditions that should assure complete destruction of organic constituents. These observations led to a deviation from the original parametric approach and the test plan was modified to identify the cause of the variability. It was suspected, and later confirmed that small amounts of organic material were migrating into the instrumentation that was above the heated reactor and not subjected to the full reaction temperature. This material would then condense and return to the reactor after cooling and contaminate the contents. Heating or removing the instrumentation and valving solved the problem. A further discussion is contained in Section 5.

4.1.2 Performance Testing

Performance testing was conducted from June 1 through June 7, 2001. During the performance testing, duplicate tests were conducted of each surrogate and the gas and liquid residuals were collected and sent to SwRI for independent analyses. The result of the testing is discussed in Sections 5 and 6.

4.2 Feeds Tested

The testing program was developed to evaluate two distinct feed materials for the batch-SCWO system – Neutralents and CAIS materiels.

4.2.1 Neutralent Materials

Two NSCMP neutralent simulants were tested. Both feed streams simulated mono-ethanolamine (MEA)-based Munitions Management Device (MMD) neutralents based on a 10:1 volume ratio of reagent to chemical agent.

The simulants were prepared using procedures that were developed by Southwest Research Institute (SwRI) of San Antonio, Texas based on these formulations[2,3].

The composition of the two simulant feeds are shown in Table 4-1.

Table 4-1 Simulant Compositions

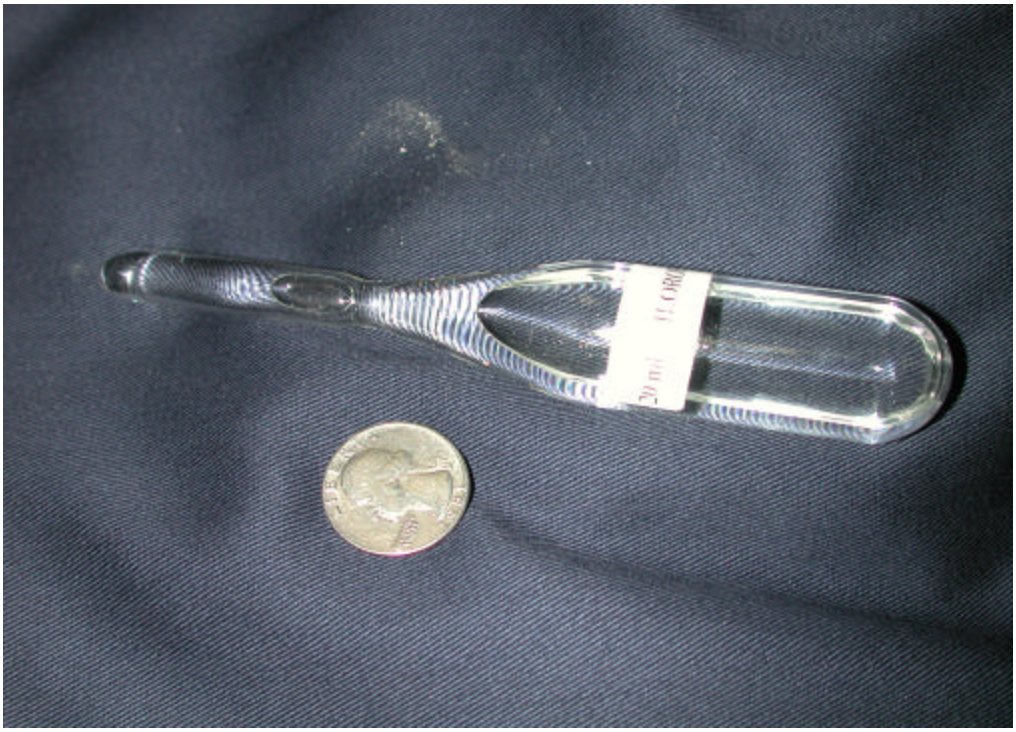
	Neutralent			Simulant		
Chemical Agent	**Major Components**	**Chemical Formula**	**Wt% in neutralent**	**Equivalent component in Simulant**	**Chemical Formula**	**Wt% in Simulant**
H Neutralent in MEA	MEA	C_2H_7NO	78	MEA	C_2H_7NO	83.00
	Water	H_2O	9.5	Water	H_2O	10.10
	MEA HCL	$C_2H_8ON\ Cl$	7.25	Dichloroethane	$C_2H_4Cl_2$	3.90
	HETM	$C_6H_{13}NOS$	5.25	Dimethyl sulfoxide	C_2H_6OS	3.00
	TOTAL		**100**			**100.00**
GB Neutralent in MEA	MEA	C_2H_7NO	38	MEA	C_2H_7NO	39.50
	Water	H_2O	50	Water	H_2O	52.00
	MEA IMP	$C_4H_{10}O_3P$	5	DMMP	$C_3H_9O_3P$	4.70
	MEA HF	$C_2H_8ON\ F$	4	Hexafluorobenzene	C_6F_6	1.60
	GB MEA	$C_6H_{15}NO_3P$	3	DMMP	$C_3H_9O_3P$	2.20
	TOTAL		**100**			**100.00**

4.2.2 CAIS Materiels

In order to test the Batch-SCWO process' ability to access the CAIS vials, a simulated CAIS vial was fabricated. The vial represented a shortened version of the K951/952 CAIS[4]. The full sized

vial would not fit in the test reactor. Therefore a shortened version was fabricated that had the same radius and wall thickness as the full-sized CAIS. The radius and wall thicknesses were maintained to ensure that the test vial required similar internal forces to break as a full-sized vial. Appendix 1 is a dimensional sketch of the simulated vial. Figure 4-1 shows a simulated CAIS vial.

Figure 4-1 Simulated CAIS Vial



Even with the smaller vial, the quantity of agent (20 ml) was too large to oxidize in the small test reactor. Consequently, the goal was not to demonstrate destruction of the chemicals, but to demonstrate that the vial would break when heated due to internal pressure build up. The ampules, were supplied by Stone and Webster and contained 20 ml of chloroform.

4.3 Test Procedure – Liquid Neutralent

Surrogate mixtures were prepared per instructions provided. Initially the chemical surrogates and caustic, if used, were loaded in the vessels before sealing the lid. After leak testing the vessel with helium, a 35-wt % solution of hydrogen peroxide was added through the valve using a hypodermic needle. Hydrogen peroxide was used as the oxidizer simply because it was easier to handle than oxygen and decomposes to oxygen and water at approximately 80 to 90 ^{o}C before the oxidation of the organic compounds begins.

Once sealed and all monitoring connections made, the vessel was placed in an insulated jacket and the band heaters energized. The heaters were physically in contact with the vessel and controlled by a feedback temperature controller that monitored the reactor internal temperature.

The vessel heatup continued until the desired temperature was reached and the timing began. After a predetermined hold/residence time, the heaters were shutoff and the insulated cans lowered, and cooling fans used to speed cooldown.

At the conclusion of each test the residual vapor was either collected in a Tedlar™ bag for analysis or vented to the fume hood. Each vessel was opened and the liquid residual was collected for analysis. During the workup tests, Sandia measured the pH of the effluent using litmus paper and total organic carbon using a Rosemount™ TOC analyzer. All samples from the performance tests were collected and sent to SwRI for independent analysis.

Figure 4-2 shows a typical pressure and temperature history. At about 500 seconds there was a rapid dissociation of hydrogen peroxide that resulted in a net pressure increase of about 100 psi and a transient temperature spike of about 100° C. This was a repeatable event that occurred on every test.

Figure 4-2 Typical Pressure and Temperature History

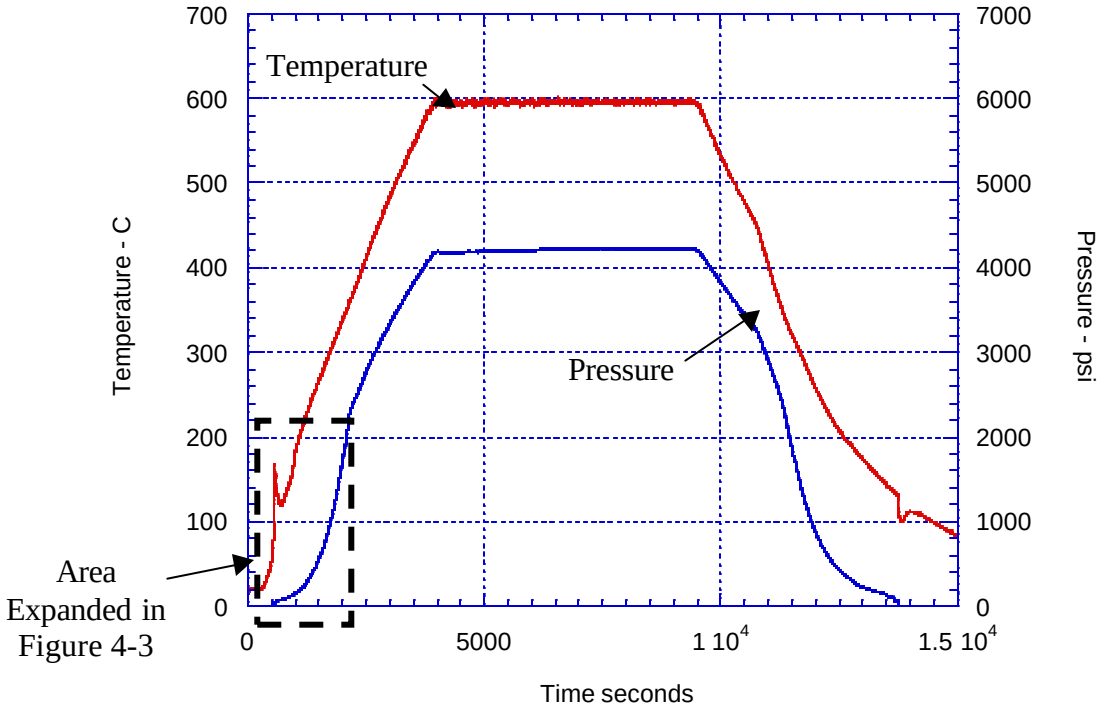
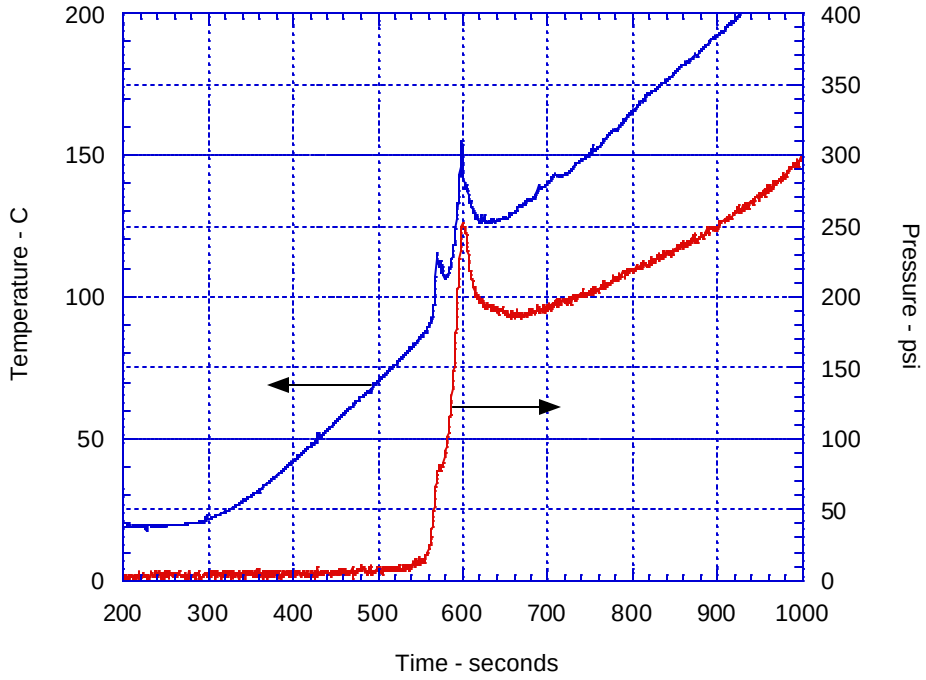


Figure 4-3 shows the dissociation reaction in higher resolution. The net pressure increase resulted from the release of oxygen that added to the partial pressure of the water. The transient temperature and pressure spike occurred because the rate of energy release exceeded the rate at which the energy could be dissipated to the vessel walls. Although the transient event was obvious, the net temperature increase was small. This is because the heat from the reaction was small compared to the total thermal energy in the vessel. The height of the spike was determined by the amount of water in the reactor. With its high thermal capacity, the water in a supercritical reactor modulates rapid reactions. More water would make the spike smaller. In these tests, the

amount of water was determined by the concentration of the hydrogen peroxide solution and was more than enough to limit the peak temperature and pressure to acceptable levels.

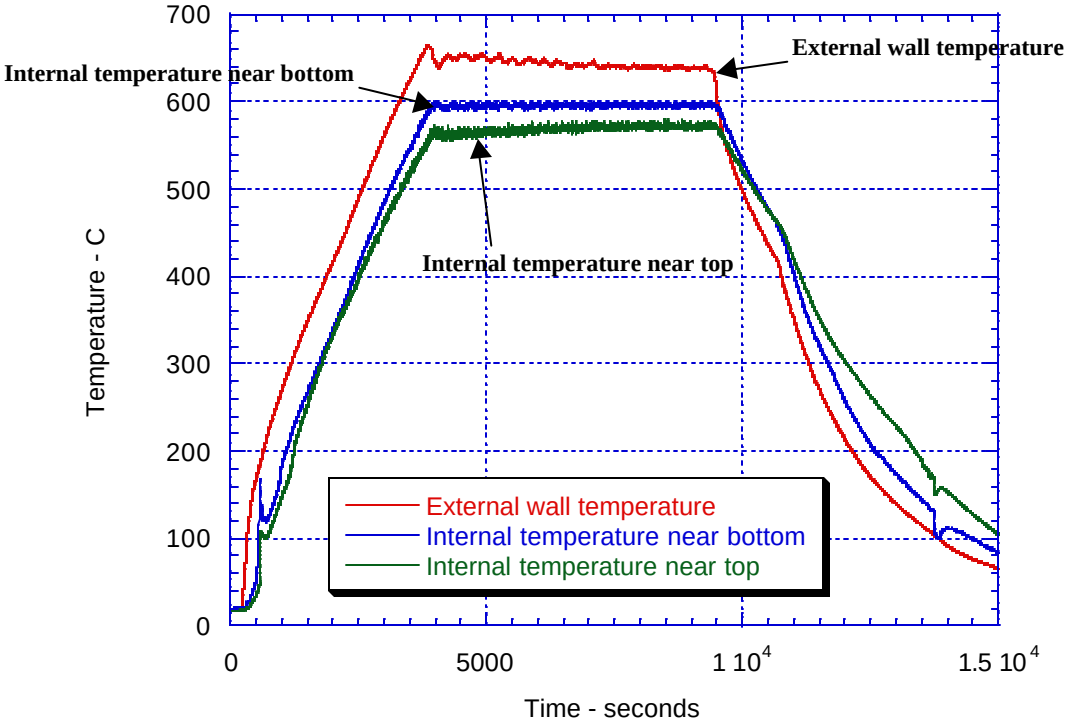
Figure 4-3 Expanded View of the Dissociation of Hydrogen Peroxide



Other than the transient event just described, the temperature and pressure climbed steadily. With some organic compounds, additional small temperature spikes may occur during the oxidation reactions, but none were observed with the compounds tested here. On the test shown in Figure 4-2, the temperature was held at 600 °C for 90 minutes. The peak temperatures and hold times varied between tests according to the test plan. After the predetermined hold/residence time, the heaters were turned off. After about 4 hours, the valve was opened to vent the overpressure from the vessel.

Temperature was controlled using the bottom internal thermocouple that was located approximately two inches off the bottom of the vessel. A second thermocouple was located near the top of the reactor, and a third on the surface of the vessel (between the heater bands and the vessel outside wall). Figure 4-4 is a plot of the three temperatures over the course of a test. The temperature at the top of the vessel was less than at the bottom because of the heat sink provided by the mass of the clamps that secure the vessel lid and because of higher heat loss due to poorer insulation. A temperature difference of about 40 °C was typical.

Figure 4-4 Temperature History at Different Locations in the Reactor



4.4 Test Procedure – CAIS

Surrogate CAIS vials were prepared by Edgewood Chemical and Biological Command (ECBC) at Aberdeen Proving Ground in accordance with a specification developed by Stone & Webster (Appendix 1) and provided to Sandia. The simulated CAIS vial was placed in an empty reactor which was sealed and leak checked with helium. Once sealed and all monitoring connections made, the vessel was placed in an insulated jacket and the band heaters energized. The heaters were physically banded directly to the vessel and controlled by a feedback temperature controller that monitors the reactor internal temperature. The vessel heatup continued while monitoring the vessel internal pressure until the simulated CAIS vial burst as indicated by an increase in pressure and temperature. In this case, no reaction of the chloroform that was in the vial occurred due to the absence of an oxidant. Once the vial burst, the heaters were shutoff and the insulated cans lowered and cooling fans are used to speed cooldown.

5. Test Results & Discussion – Liquid Neutralents

The performance testing clearly indicated that when processing liquid neutralent at 600 ^{o}C with a hold/residence time of one hour, the liquid residue consistently contains less than 10 ppm TOC. However, due to complications encountered during the testing, little is known of the kinetics of the reaction, including whether operating at a lower temperature could yield similar results. On the positive side, the testing did provide a universal processing condition that may be applied to liquid neutralents.

The following section discusses the results of the workup and performance testing that was conducted in this program (Sections 5.1 and 5.2, respectively). That is followed by a discussion of the general operability of the Batch-SCWO process and its practicality/applicability for use in the NSCMP (Section 5.3). Section 5.4 and 5.5 are summaries of the analytical results.

5.1 Workup Testing

Workup testing commenced on April 10, 2001 and continued through May 30, 2001. A total of 45 tests were conducted on H and GB simulant at temperatures ranging from 300 to 600 ^{o}C and hold residence times of 0 to 120 minutes. Table 5-1 is a summary of the testing that was conducted in this program[5]. Initially the goal was to develop an understanding of the dependence of destruction efficiency (measured as residual TOC) vs. time and temperature. However it was noted early that the results were inconsistent and even appeared random. For example, during test number 18 conducted on April 20, no organic material was loaded and the resulting TOC was 43 ppm.

Sandia suspected that small amounts of organic material were migrating into the dead volumes in the instrumentation and valves located on top of the reactor (see Figures 3-1 and 3-2). Since these areas were not heated the material would not oxidize and, once the reactors cooled, the material would condense and flow back into the reactor, contaminating the contents.

Sandia first attempted to extend the heated area to include these dead volumes, through the use of heat tape (test runs 14, 20, 22-25). However, the pressure transducers and valve stem and packing were not rated for SCWO temperatures. The valves were heated to between 300 and 400^{o}C, but the transducers were not heated. This resulted in some improvement, but did not fully resolve the problem. Furthermore, with the valves near their temperature limit there were increased instances of leaks in the valve. Nearly 10% of the workup tests were aborted due to leaking valves once heat tape was applied.

Examination of the internal designs of the external piping indicated that the probable cause of material hang-up was the pressure transducer since it extended horizontally and provided a convenient dead volume for material to collect. The pressure transducer was removed starting with run 28, and with the valve heated, the residual TOC's were consistently less than 10 ppm.

Once the equipment problems were solved, the system performed consistently and Sandia selected an operating temperature of 600 ^{o}C and a hold/residence time of 60 minutes as their operating conditions for the performance test.

Table 5-1 Test Matrix

Number	Date	Intent	Agent ID	NaOH	°C	Hold time (min)	Psi	TOC Sandia (ppm)	TOC SwRI (ppm)	pH	Comments
Workup Testing											
1	4/10/01	Oxidize GB simulant at different times/temperatures	GB/MEA	No	N/A	N/A	N/A	N/A	N/A	N/A	Aborted due to heater problems
2	4/10/01		GB/MEA	No	400	0	2800	734	N/A	7	
3	4/10/01		GB/MEA	No	500	0	3800	135	N/A	8	
4	4/10/01		GB/MEA	No	600	30	4300	24	N/A	N/A	
5	4/11/01		GB/MEA	No	300	30	1400	1506	N/A	N/A	
6	4/11/01		GB/MEA	No	300	0	1300	6693	N/A	N/A	
7	4/17/01	Prove destruction. All vessels at 600 C. Different hold times.	GB/MEA	No	600	90	4225	6	N/A	N/A	
8	4/17/01		GB/MEA	No	600	120	4450	23	N/A	N/A	
9	4/17/01		GB/MEA	No	600	30	4380	37	N/A	N/A	
10	4/17/01		GB/MEA	No	600	60	4760	9	N/A	N/A	
11	4/18/01	Excess oxidizer	GB/MEA	No	600	30	4390	8	N/A	N/A	
12	4/18/01	Insulate top	GB/MEA	No	600	30	4670	10	N/A	N/A	
13	4/18/01	Add caustic	GB/MEA	Yes	600	30	4800	7	N/A	N/A	
14	4/18/01	Heat tape on valve	GB/MEA	No	N/A	N/A	N/A	N/A	N/A	N/A	Aborted due to valve leak
15	4/19/01	Oxidize H simulant at different temperatures	H/MEA	Yes	400	30	2400	110	N/A	N/A	
16	4/19/01		H/MEA	Yes	500	30	3400	158	N/A	N/A	
17	4/19/01		H/MEA	Yes	600	30	4300	14	N/A	N/A	

N/A – Not Analyzed

Table 5-1 Test Matrix (cont)

Number	Date	Intent	Agent ID	NaOH	°C	Hold time (min)	Psi	TOC Sandia (ppm)	TOC SwRI (ppm)	pH	Comments
Workup Testing (cont)											
18	4/20/01	No organic	none	Yes	600	60	4100	43	N/A	N/A	
19	4/20/01	Look at repeatability	GB/MEA	Yes	600	60	4700	42	N/A	N/A	
20	4/20/01	Heated valve	GB/MEA	Yes	600	60	5100	39	N/A	N/A	
21	4/20/01	Look at repeatability	H/MEA	Yes	600	30	4350	43	N/A	N/A	Loaded on 4/19/01. Tested on 4/20/01
22	4/30/01	Heat tape on valve,	GB/MEA	Yes	600	60	N/A	38	9.37	8	Samples combined for TOC analysis at SwRI to improve accuracy
23	4/30/01		GB/MEA	Yes	600	60	N/A	35	9.37	7.5	
24	4/30/01		H/MEA	Yes	600	60	N/A	N/A	N/A	N/A	Vessels were loaded with incorrect quantities
25	4/30/01		H/MEA	Yes	600	60	N/A	N/A	N/A	N/A	
26	5/1/01	Repeat failed tests from 4/30/01	H/MEA	Yes	600	60	N/A	N/A	64.2	6	Samples combined for TOC analysis at SwRI to improve accuracy
27	5/1/001		H/MEA	Yes	600	60	N/A	N/A	64.2	9	
28	5/8/01	Remove transducer to improve destruction	H/MEA	Yes	N/A	N/A	N/A	N/A	N/A	N/A	Aborted due to control system malfunction
29	5/8/01		H/MEA	Yes	N/A	N/A	N/A	N/A	N/A	9	Aborted due to valve leak
30	5/8/01		H/MEA	Yes	600	60	N/A	1.5	N/A	5	
31	5/8/01		H/MEA	Yes	600	60	N/A	5.1	N/A	4	
32	5/14/01	Collect samples for SwRI analysis	GB/MEA	Yes	600	60	N/A	N/A	5.17	8	Gas and liquid sample analyzed by SwRI
33	5/14/01		GB/MEA	Yes	N/A	N/A	N/A	N/A	N/A	N/A	Aborted due to control system malfunction
34	5/14/01		H/MEA	Yes	N/A	N/A	N/A	N/A	N/A	N/A	
35	5/14/01		H/MEA	Yes	N/A	N/A	N/A	N/A	N/A	N/A	

N/A – Not Analyzed

Table 5-1 Test Matrix (cont)

Number	Date	Intent	Agent ID	NaOH	°C	Hold time (min)	Psi	TOC Sandia (ppm)	TOC SwRI (ppm)	pH	Comments
Workup Testing (cont)											
36	5/18/01	Collect gas and liquid samples for SwRI	GB/MEA	Yes	600	60	N/A	N/A	N/A	8	Gas samples leaked
37	5/18/01		GB/MEA	Yes	N/A	N/A	N/A	N/A	N/A	N/A	Aborted due to heater failure
38	5/18/01		H/MEA	Yes	N/A	N/A	N/A	N/A	N/A	N/A	Aborted due to valve leak
39	5/18/01		H/MEA	Yes	600	60	N/A	N/A	N/A	5	
40	5/21/01	Repeat 5/18/01 #1	GB/MEA	Yes	600	60	N/A	N/A	1	8.5	Gas sample analyzed by SwRI
41	5/21/01	Break simulated CAIS ampules	Sim. CAIS	No	N/A	N/A	N/A	N/A	N/A	N/A	Vial opened at 235 °C
42	5/21/01		Sim CAIS	No	N/A	N/A	N/A	N/A	N/A	N/A	Vial opened at 242 °C
43	5/21/01		Sim CAIS	No	N/A	N/A	N/A	N/A	N/A	N/A	Vial opened at 248 °C
44	5/23/01	Remove transducers and heat valves. Test at different temperatures.	H/MEA	Yes	525	60	N/A	N/A	1	7	Gas sample analyzed by SwRI
45	5/23/01		H/MEA	Yes	N/A	N/A	N/A	N/A	N/A	N/A	Aborted due to valve leak
46	5/23/01		H/MEA	Yes	N/A	N/A	N/A	N/A	N/A	N/A	
47	5/23/01		H/MEA	Yes	600	60	N/A	N/A	1	5	Gas sample analyzed by SwRI
48	5/30/01	Remove transducers	GB/MEA	Yes	600	60	N/A	N/A	N/A	8	
49	5/30/01		GB/MEA	Yes	600	60	N/A	N/A	N/A	9	
50	5/30/01	Simulated CAIS ampule	Sim CAIS	No	N/A	N/A	N/A	N/A	N/A	N/A	Vial opened at 240 °C
51	5/30/01	Simulated CAIS w/ H_2O_2	Sim CAIS	No	N/A	N/A	N/A	N/A	N/A	N/A	Vial opened at 256 °C

N/A – Not Analyzed

Table 5-1 Test Matrix (cont)

Number	Date	Intent	Agent ID	NaOH	°C	Hold time (min)	Psi	TOC Sandia (ppm)	TOC SwRI (ppm)	pH	Comments
Performance Test											
P-1	6/1/01	Demonstrate destruction	GB/MEA	Yes	600	60	N/A	N/A	1	7	Sample to SwRI
P-2	6/1/01		GB/MEA	Yes	600	60	N/A	N/A	1	7	Sample to SwRI
P-3	6/1/01	Simulated CAIS	Sim. CAIS	No	N/A	N/A	N/A	N/A	N/A	N/A	Vial opened at 280 °C
P-4	6/1/01	Simulated CAIS w/ H_2O_2	Sim CAIS	No	N/A	N/A	N/A	N/A	N/A	N/A	Vial opened at 240 °C
P-5	6/4/01	Demonstrate destruction	H/MEA	Yes	600	60	N/A	N/A	3.14	8	Sample to SwRI
P-6	6/4/01		H/MEA	Yes	600	60	N/A	N/A	1	10	Sample to SwRI
P-7	6/4/01	Small vial w/ H_2O	H_2O	No	N/A	N/A	N/A	N/A	N/A	N/A	Screw top bottle
P-8	6/4/01	H_2O_2 only	N/A	No	N/A	N/A	N/A	N/A	N/A	N/A	To clean vessel
P-9	6/5/01	Test at 550 °C	GB/MEA	Yes	550	60	N/A	N/A	1	N/A	Sample to SwRI
P-10	6/5/01		GB/MEA	Yes	550	60	N/A	N/A	N/A	N/A	Aborted due to valve leak
P-11	6/5/01		H/MEA	Yes	550	60	N/A	N/A	18	N/A	Sample to SwRI
P-12	6/5/01		H/MEA	Yes	N/A	N/A	N/A	N/A	N/A	N/A	Aborted due to valve leak
P-13	6/6/01	Demonstrate destruction	GB/MEA	Yes	600	60	N/A	N/A	1	N/A	Sample to SwRI
P-14	6/6/01		GB/MEA	Yes	N/A	N/A	N/A	N/A	N/A	N/A	Aborted due to valve leak
P-15	6/6/01		H/MEA	Yes	N/A	N/A	N/A	N/A	N/A	N/A	Aborted due to valve leak
P-16	6/6/01		H/MEA	Yes	600	60	N/A	N/A	1	N/A	Sample to SwRI
P-17	6/7/01	Demonstrate repeatability	GB/MEA	Yes	600	60	N/A	N/A	1.9	N/A	Sample to SwRI
P-18	6/7/01	no valve	GB/MEA	Yes	600	60	N/A	N/A	1	N/A	Sample to SwRI
P-19	6/7/01	no valve	H/MEA	Yes	600	60	N/A	N/A	4.7	N/A	Sample to SwRI
P-20	6/7/01	Demonstrate repeatability	H/MEA	Yes	600	60	N/A	N/A	1	N/A	Sample to SwRI

N/A – Not Analyzed

5.2 Performance Testing

On June 1, 2001 the performance test was initiated. The purpose of the performance test was to conduct an independent evaluation of the Batch-SCWO process including analysis of the residuals and evaluate the performance against pre-defined criteria.

Twenty tests were initiated, and sixteen completed using simulated H and GB neutralent as shown in Table 5-2.

Table 5-2 Performance Tests

Number	Date	Simulant	Temp °C	Hold time (min)	TOC (ppm)	Weight (g)	Volume (mL)	Gas Sample	Liquid Sample	Comments
P-1	6/01/01	GB/MEA	600	60	< 1.0	30.53	29.6	yes	yes	
P-2	6/01/01	GB/MEA	600	60	< 1.0	32.34	30.9	yes	yes	
P-5	6/04/01	H/MEA	600	60	3.14	27.26	25.6	yes	yes	
P-6	6/04/01	H/MEA	600	60	< 1.0	39.66	36.8	yes	yes	
P-9	6/05/01	GB/MEA	550	60	< 1.0	28.89	29.1	yes	yes	
P-10	6/05/01	GB/MEA	550	60	N/A	N/A	N/A	N/A	N/A	Aborted due to valve leak
P-11	6/05/01	H/MEA	550	60	18	24.23	24.4	yes	yes	
P-12	6/05/01	H/MEA	550	60	N/A	N/A	N/A	N/A	N/A	Aborted due to valve leak
P-13	6/06/01	GB/MEA	600	60	< 1.0	27.57	27.7	yes	yes	
P-14	6/06/01	GB/MEA	600	60	N/A	N/A	N/A	N/A	N/A	Aborted due to valve leak
P-15	6/06/01	H/MEA	600	60	N/A	N/A	N/A	N/A	N/A	Aborted due to valve leak
P-16	6/06/01	H/MEA	600	60	< 1.0	24.35	24.5	yes	yes	
P-17	6/07/01	GB/MEA	600	60	1.91	28.58	28.8	yes	yes	
P-18	6/07/01	GB/MEA	600	60	< 1.0	29.63	30.3	N/A	yes	Valve Removed
P-19	6/07/01	H/MEA	600	60	4.43	24.66	24.4	N/A	yes	Valve Removed
P-20	6/07/01	H/MEA	600	60	< 1.0	18.67	18.9	yes	yes	

N/A – Not Analyzed

Tests on the first and second day were conducted at 600 °C with a 60-minute hold/residence time for H and GB. On the third day Sandia was requested to conduct a test at 550 °C to evaluate the system performance at a lower temperature. During that test problems were encountered with leaking valves on two of the four reactors and it was determined that efforts should focus on completing the validation of Sandia's preferred operating conditions prior to embarking on other objectives.

The fourth day was planned to be a test of simulated GB and H neutralent to repeat the tests of the first and second day. That would have completed the performance testing by providing duplicate tests of the optimal operating conditions. Two of the four repeatability tests planned for day four were aborted due to leaking valves, and the testing was extended an additional day.

Since adequate gas samples had been obtained, it was decided to remove the valve on the two reactors that leaked the previous day and conduct a final validation test at 600 ^{o}C and 60-minutes. This test was completed and liquid samples collected for analysis.

While the valves failed during the performance tests resulting in aborting 25 % of the tests, this is not considered a significant problem. The valves that were used for this test program were part of the original stock at Sandia from previous testing and it was thought that their reuse would not cause a problem. However, the challenge of consistently achieving 10 ppm TOC in the residual turned out to be more difficult than anticipated. This was the first time that Sandia was challenged to achieve that level of destruction, and the first time they had to heat the reactor externals.

The fact that this problem was encountered, identified and solved at the bench scale is good. It is now recognized that the full-scale system must be designed with valves and instrumentation that will minimize dead volumes where material can collect and be capable of withstanding the SCWO temperatures. Materials and components meeting these specifications are available in the commercial market.

5.3 Operability

The Batch-SCWO bench-scale unit generally operated well other than the problems with the external valves and instrumentation dead legs that were noted previously. With the proper design and choice of equipment, these problems should be eliminated.

All testing was conducted on the bench-scale system, and the equipment and operations, while similar, were not entirely prototypical of a full-scale system, however the unit did incorporate many of the features that would be a part of a full-scale system. These are discussed in the following section while the features of a full-scale processing concept are discussed in Section 7.

5.3.1 System Operation

The bench-scale Batch-SCWO system operation was simple. The material was loaded into the cold reactor and sealed, the system was leak checked, and the heater control system energized. Four reactor systems were operated simultaneously all capable of independent control. In nearly all cases, the heatup and maintenance of reaction temperature proceeded without incident. Temperature and pressure (although later the transducer was removed) were recorded by the data acquisition system and accurate plots of the system operation were available.

Heatup to 600 ^{o}C generally took about one-hour. At the completion of the hold/residence time, the heaters were de-energized and the insulating “cans” were lowered from around the reactor and fans energized to cool the reactors by convection. Approximately two-hours were required to cool the reactors prior to depressurizing and removing the head.

The test effectively demonstrated the mechanical process of Batch-SCWO as it would be applied in a full-scale system.

5.3.2 Graylock™ seals

The Graylock™ seals used in the bench-scale unit are essentially the same that would be in a larger unit, although the method of securing the clamping mechanism may be different (mechanically assisted) in a larger unit. In more than 70 completed tests, there was not a single leak attributed to the Graylock™ seal. The operator noted that regular replacement of the seal ring after 3 to 5 runs was critical to achieving reliable seals.

5.3.3 External heaters

The bench-scale system was heated with commercially available external band heaters. These were purchased as catalog items and fitted to the vessels. They were able to bring the small reactors up to temperature and hold at the desired setpoint well. The bench vessels were heated only on the lower portion and the head and clamping mechanism insulated. In a full-scale system, a more extensive heating system would be required to heat the vessel head and clamping mechanism and maintain the system temperature.

5.3.4 External valving

The valves used in the bench apparatus were existing stock at Sandia. They had been used in previous SCWO work and Sandia determined that they were adequate for the application. In previous applications the valves were isolated from the reaction conditions and functioned as anticipated. The valves also functioned in the beginning of this program. However, as the problems with material migrating into the external areas was discovered, the readily apparent solution was to heat the valves and thereby ensure that reaction would occur even in these areas. The valve and tubing were heat taped and maintained at a temperature of approximately 400 to 450 ^{o}C to encourage reaction.

Once the valves were heated, problems with leaking were observed. As the valves were investigated, it was determined that the packing needed to be changed to a material more stable at higher temperatures, this was completed. However, it was later determined that the valve stem was at the limit of its rated temperature and a probable cause of leakage.

While valve leaks were a chronic problem throughout the performance test, it was a valuable observation for scale-up of the system. A key design goal in the full-size application will be to minimize the unheated volume of any sample tubing and valving. In addition, particular care will have to be given to procuring valves that are rated for SCWO conditions.

5.3.5 Instrumentation

Instrumentation in the test apparatus included thermocouples for temperature monitoring installed in the vessel (2) and on the exterior side. The internal thermocouples were installed through the vessel head and in Inconel 600™ sheaths. The internal thermocouples sensed temperature in the top and lower third of the reactor. The lower sensing element was used to control the external heaters. The thermocouples functioned as designed.

Pressure was monitored initially in all reactors using a pressure transducer that was mounted in the line between the vessel head and sample valve. The transducer model that was used

projected horizontally from the vertical tubing and it appeared that this horizontal leg provided a convenient place for some reaction material to "hide" from the full reaction temperature. As in the case with valves, the design of a full-scale system must consider minimizing the potential for any material to migrate into an area where it would not be exposed to reaction conditions. Commercial transducers are available that are better suited for this application.

5.3.6 Control and Data Acquisition

Each Batch-SCWO reactor heater was controlled by an independent programmable controller. The instrumentation was input into a standard PC-based data acquisition system (Odyssey 966™). A full-scale system would probably include an integrated control/data acquisition system that was PC-based. The independent bench-scale system was used for flexibility and because it was less expensive. While the bench-scale system functioned well for the testing, the disadvantage of the setup is that the data acquisition system is independent of any control function and therefore has no record of the setpoints or control parameters.

The integrated control/data acquisition of a system such as a Batch-SCWO system is straightforward and can be accomplished by a variety of commercially available programs.

5.4 Feed Analysis

Feeds were prepared in accordance with the provided procedures that were developed by SwRI[6,7]. At the time of the performance test, a sample of the simulated neutralent was analyzed. In addition a separate analysis was conducted of the reactor vessel mixture that represented the mixed simulant, oxidant and caustic prior to heatup.

5.4.1 Simulant analysis

Table 5-3 presents the NMR, anion, and TOC analyses of the neutralent simulant samples submitted by Sandia to SwRI. The accuracy of the NMR analyses, utilizing protocols developed by SwRI, is $\pm$ 5 percent.

The "DMMP reaction byproduct" could not be identified by the NMR analysis. However, SwRI reported that it was a similar compound that contained a Carbon-Phosphorous bond. The NMR also failed to detect hexafluorobenzene, which according to the feed specifications should have been present at a level of 1.6 percent by weight in the GB neutralent simulant.

An analysis of the simulant mixture for "free" fluoride ions by ion chromatography was conducted. The result, shown in Table 5-3, is non-detectable levels of fluoride. The analytical absence of detectable fluoride was suspect since theoretically there should be approximately 9,000 ppm in the simulant mixture. To measure the total fluoride, the GB neutralent simulant was analyzed utilizing EPA SW-846 Method 5050, "Bomb Preparation Method for Solid Waste." In this method a sample is oxidized by combustion in a bomb (Parr Oxygen Bomb™, P/N 1108) containing oxygen under pressure. The liberated compounds are absorbed in a sodium carbonate/sodium bicarbonate solution. The liquid residual was then analyzed for fluoride using an ion selective electrode. The results of this analysis are also presented in Table 5-3 and indicate a fluoride concentration of 103 ppm (an average of two analyses).

It is not known why the fluoride concentration is significantly less than predicted. SwRI suspects that the density difference between the hexafluorobenzene (specific gravity = 1.6) and MEA (specific gravity = 1.0) may have caused concentration gradients during storage and the simulant mixture may not have been thoroughly mixed prior to collecting the sample. More care will be required in future programs to ensure that the samples used in testing are representative.

Table 5-3 Simulant Analysis [8]

	H Neutralent in MEA		GB Neutralent in MEA	
Analyte	**SwRI**	**Theoretical**	**SwRI**	**Theoretical**
Monoethanolamine, MEA (%wt)	86	83	41	39.5
Dichloroethane, DCE (%wt)	7	3.9	N/A	N/A
Dimethyl sulfoxide, DMSO (%wt)	5	3	N/A	N/A
Dimethyl methylphosphonate, DMMP (%wt)	N/A	N/A	4	6.9
"DMMP reaction byproduct" (1) (%wt)	N/A	N/A	3	N/A
Hexafluorobenzene (%wt)	N/A	N/A	< 1	1.6
TOC, mg/L	354,000	345,300	189,500	181,600
Fluoride, mg/L (by ion chromo) (2)	< 10	N/A	< 10	9,800
Fluoride, mg/L (by bomb cal) (3)	N/A	N/A	103	9,800
Chloride, mg/L	21,341	27,600	< 10	N/A

N/A – Not Analyzed

(1) "DMMP Reaction Product" could not be specifically identified, however it is similar in structure to DMMP containing a C-P bond.[9]

(2) Fluoride analyzed using EPA SW-846 Method 9056, "Determination of Inorganic Anions by Ion Chromatograph."

(3) Fluoride analyzed using EPA SW-846 Method 5050, "Bomb Preparation Method for Solid Waste."

5.4.2 Reactor Content Analysis

It was observed that when mixing the simulant, hydrogen peroxide and caustic in the reactor vessel, a reaction would occur. A test was conducted at SwRI where a mixture of the initial reactor contents was prepared based on Sandia's instructions and analyzed to determine if any oxidation of the feed materials occurred in the absence of any heating.

Aliquots of the GB and H neutralent simulants provided to SwRI were mixed with the appropriate quantities of sodium hydroxide and hydrogen peroxide to represent the feed solutions for the Batch SCWO process. The "recipes" provided to SwRI for simulating the reactor feeds were as follows:

- H reactor recipe
  - 2.0 grams of H neutralent simulant
  - 0.5 grams of 40 percent sodium hydroxide

  - 28.2 grams of 35 percent hydrogen peroxide
- GB reactor recipe
  - 4.0 grams of GB neutralent simulant
  - 1.1 grams of 40 percent sodium hydroxide
  - 29.9 grams of 35 percent hydrogen peroxide

Initial attempts to obtain valid samples of the two feed solutions were complicated by the vigorous reaction that occurred for several hours after the components were mixed. For example, a three-fold batch of each recipe (i.e., approximately 100 grams of material) placed into a 1-Liter flask boiled over into the laboratory hood containing the flasks. The reaction was not immediate; the temperature of the solution gradually increased, accompanied by the release of gas bubbles, until the solution eventually overflowed the container.

A double batch of each recipe (61.4 grams of H and 70.0 grams of GB) was placed into individual 2-Liter flasks. Over a period of several hours, the solutions were allowed to react until the bubbling subsided and it was safe to place the solutions into closed sample containers. No liquid material boiled out of flask, however, the reaction did generate gases that caused a reduction in the original mass of the liquid solutions. The quantities of each liquid recipe recovered from the flasks were: 50.7 grams of H (82.6 percent) and 59.6 grams of GB (85.1 percent).

These samples were analyzed for TOC and by NMR. These results were compared to the expected component concentrations based on the planned theoretical as well as that based on the actual simulant analysis (see Table 5-3). As shown in Table 5-4, the reactor feeds showed no change (within the $\pm$ 5 percent limit of the NMR technique) from the original, raw simulant based upon the expected dilution by the other materials. Dichloroethane was not detectable in the H reactor solution. The energetic reaction observed subsequent to the mixing of the simulants, caustic, and hydrogen peroxide is primarily attributable to the degradation of the hydrogen peroxide in the highly alkaline solutions and the release of oxygen. The heat of this reaction, and possibly some oxidation by the hydrogen peroxide, could be reasonably expected to cause the minor reductions in the simulant components.

Table 5-4 Initial Reactor Contents Analysis

	H Neutralent + Oxidant			GB Neutralent + Oxidant		
Analyte	**Theoretical (1)**	**Theoretical (2)**	**SwRI Analysis**	**Theoretical (1)**	**Theoretical (2)**	**SwRI Analysis**
Simulant (g)	2.0	N/A	N/A	4.0	N/A	N/A
35 % Hydrogen Peroxide (g)	28.2	N/A	N/A	29.9	N/A	N/A
40 % Sodium Hydroxide (g)	0.5	N/A	N/A	1.1	N/A	N/A
Monoethanolamine, MEA (%wt)	5.4	5.6	5.1	4.5	4.7	3.0
Dichloroethane, DCE (%wt)	0.3	0.5	< 0.1	N/A	N/A	N/A
Dimethyl sulfoxide, DMSO (%wt)	0.2	0.3	0.4	N/A	N/A	N/A
Dimethyl methylphosphonate, DMMP (%wt)	N/A	N/A	N/A	0.8	0.54	0.52
DMMP "byproduct" (%wt)	N/A	N/A	N/A	N/A	0.40	0.39
Total Organic Carbon (ppm)	22,495	23,062	22,800	20,754	21,657	21,600

N/A – Not Analyzed
(1) Theoretical concentration based on mixture recipe (see Table 4-1)
(2) Theoretical concentrations based on actual simulant analysis (see Table 5-2)

5.5 Residual characteristics

All residuals from the performance test were collected and analyzed in accordance with the Sampling and Analysis Plan. The results reported herein are based on the report received from the analytical subcontractor (SwRI) [10]. A copy of the summary report is included as Appendix 2 in this report.

5.5.1 Gases

The residual gases from the performance tests were collected in Tedlar™ bags and sent to SwRI for analysis. The samples were analyzed as summarized in Table 5-5.

5.5.1.1 Permanent Gases and Carbon Monoxide

These analyses were performed in accordance with SwRI TAP 01-0405-013 (Rev1/Sep 00) on two analytical sequences by using a 5A Mol Sieve column in conjunction with a PDHID detector for the carbon monoxide. A TCD detector was used in conjunction with an Alltech CTRI™ column for the remaining gases. Table 5-6 presents gas concentrations measured in the samples. For carbon monoxide, a detection limit of 100 ppmv was obtained and none of the samples contained this compound at this limit. In order to obtain the best possible accuracy, the standards as well as the samples were run in duplicate to assure reproducibility and the average was used to calculate the concentration.

Table 5-5 Gas Sample Analyses

Num.	Date	Simulant	Temp °C	Time (min)	Liquid TOC (ppm)	Gas Analyses Performed			
						Permanent Gases	Inorganic Gases	Semi- VOC	VOC
P-1	**6/01/01**	GB/MEA	600	60	< 1.0	XX	N/A	XX	XX
P-2	**6/01/01**	GB/MEA	600	60	< 1.0	N/A	XX	N/A	N/A
P-5	**6/04/01**	H/MEA	600	60	3.14	N/A	XX	N/A	N/A
P-6	**6/04/01**	H/MEA	600	60	< 1.0	XX	N/A	XX	XX
P-9	**6/05/01**	GB/MEA	600	60	< 1.0	XX	N/A	N/A	XX
P-10	**6/05/01**	H/MEA	550	60	18	XX	N/A	N/A	XX
P-13	**6/06/01**	GB/MEA	600	60	< 1.0	XX	N/A	XX	XX
P-16	**6/06/01**	H/MEA	600	60	< 1.0	XX	N/A	XX	XX
P-17	**6/07/01**	GB/MEA	600	60	1.91	N/A	XX	N/A	N/A
P-18	**6/07/01**	GB/MEA	600	60	< 1.0	Valve removed no gas sample obtained			
P-19	**6/07/01**	H/MEA	600	60	4.43	Valve removed no gas sample obtained			
P-20	**6/07/01**	H/MEA	600	60	< 1.0	N/A	XX	N/A	N/A

XX = Analyses performed
N/A = Not analyzed

Table 5-6 Permanent Gases and Carbon Monoxide Results.

Num.	Date	Simulant	Temp (°C)	Time (min)	Liquid TOC (ppm)	CO2 (%)	O2 (%)	N2 (%)	CO (ppmv)
P-1	**6/01/01**	GB/MEA	600	60	< 1.0	32.1	42.7	15.7	< 100
P-2	**6/01/01**	GB/MEA	600	60	< 1.0	N/A	N/A	N/A	N/A
P-5	**6/04/01**	H/MEA	600	60	3.14	N/A	N/A	N/A	N/A
P-6	**6/04/01**	H/MEA	600	60	< 1.0	14.7	59.4	17.5	< 100
P-9	**6/05/01**	GB/MEA	600	60	< 1.0	33.9	43.2	12.3	< 100
P-10	**6/05/01**	H/MEA	550	60	18	35.8	37.8	15.1	< 100
P-13	**6/06/01**	GB/MEA	600	60	< 1.0	31.2	41.7	17.1	< 100
P-16	**6/06/01**	H/MEA	600	60	< 1.0	28.6	44.3	17.2	< 100
P-17	**6/07/01**	GB/MEA	600	60	1.91	N/A	N/A	N/A	N/A
P-18	**6/07/01**	GB/MEA	600	60	< 1.0	Valve removed no gas sample obtained			
P-19	**6/07/01**	H/MEA	600	60	4.43	Valve removed no gas sample obtained			
P-20	**6/07/01**	H/MEA	600	60	< 1.0	N/A	N/A	N/A	N/A

N/A = Not analyzed

5.5.1.2 Inorganic Gas Analysis

The analytical results of the gases collected in the Tedlar sample bags for various inorganic analytes are presented in Table 5-7. The analytes include sulfur dioxide (SO_2), chlorine (Cl_2),

nitric oxide (NO), nitrogen dioxide (NO_2), sulfuric acid (H_2SO_4), hydrogen chloride (HCl), and hydrogen fluoride (HF). The gases within the Tedlar samples bags were extracted through the appropriate filters, sorbent tubes, or impinger solutions as detailed in the Sampling and Analysis Plan. With the exception of trace quantities of hydrogen chloride found in one of the samples, the masses of all the other analytes in the samples were below the reported detection limits.

Table 5-7 Inorganic Gas Analyses

Num.	Date	Simulant	Temp (°C)	Time (min)	Liquid TOC (ppm)	Mass of Compound detected (total micrograms)						
						SO_2	Cl_2	NO	NO_2	H_2SO_4	HCl	HF
P-1	**6/01/01**	GB/MEA	600	60	< 1.0	N/A	N/A	N/A	N/A	N/A	N/A	N/A
P-2	**6/01/01**	GB/MEA	600	60	< 1.0	N/A	N/A	< 1.3	< 1.3	N/A	N/A	< 1.6
P-5	**6/04/01**	H/MEA	600	60	3.14	< 2.0	< 5.2	< 1.3	< 1.3	< 2.0	**1.3**	N/A
P-6	**6/04/01**	H/MEA	600	60	< 1.0	N/A	N/A	N/A	N/A	N/A	N/A	N/A
P-9	**6/05/01**	GB/MEA	600	60	< 1.0	N/A	N/A	N/A	N/A	N/A	N/A	N/A
P-10	**6/05/01**	H/MEA	550	60	18	N/A	N/A	N/A	N/A	N/A	N/A	N/A
P-13	**6/06/01**	GB/MEA	600	60	< 1.0	N/A	N/A	N/A	N/A	N/A	N/A	N/A
P-16	**6/06/01**	H/MEA	600	60	< 1.0	N/A	N/A	N/A	N/A	N/A	N/A	N/A
P-17	**6/07/01**	GB/MEA	600	60	1.91	N/A	N/A	< 1.3	< 1.3	N/A	N/A	< 1.6
P-18	**6/07/01**	GB/MEA	600	60	< 1.0	Valve removed no gas sample obtained						
P-19	**6/07/01**	H/MEA	600	60	4.43	Valve removed no gas sample obtained						
P-20	**6/07/01**	H/MEA	600	60	< 1.0	< 2.0	< 6.5	< 1.3	< 1.3	< 2.0	< 1.0	N/A

N/A = Not analyzed

5.5.1.3 Gas Analysis for Semi-Volatile Organic Compounds

The gases collected in the Tedlar sample bags were extracted through a XAD-2 resin sorbent and analyzed for semi-volatile organic compounds utilizing EPA Method 8270. The analyses looked for 75 specific compounds that are listed in the analytical report contained in Appendix 2. Only two compounds, butylbenzylphthalate and bis (2-Ethylhexyl) phthalate, were found above their respective detection limit. The masses of these two compounds were nearly identical in all of the samples. Phthalate compounds are common contaminants associated with synthetic polymeric compounds. It is strongly suspected that the presence of these two compounds in the samples are due to sample contamination from the Tedlar sample bags, or the Tygon tubing used in the analysis rather than being actual constituents of the exhaust gases.

5.5.1.4 Gas Analysis for Volatile Organic Compounds

The gases collected in the Tedlar sample bags were analyzed for their VOC content using EPA Method TO-14. Table 5.4-4 presents the results of the analyses. Since a known aliquot volume of gas was directly injected from the sample bag into the GC/MS, the concentrations of the VOC compounds could be calculated and represent the concentrations in the original gas sample. The

62 compounds presented in the table are target compounds specified by the EPA Method TO-14 that are positively identified by the method protocol.

The summary table indicates that a variety of compounds were detected in trace quantities in the residual gas. In some cases the compounds may be contaminants, but the fact that the detected compounds are present in greater quantities in the sample from the simulated H neutralent collected on June 5 (processed at a lower temperature) indicates that they are probably actual residuals. However, all compounds detected at the 600 ^{o}C tests are present at very low quantities and do not pose an immediate obstacle to potential permitting of a system.

Table 5-8 Volatile Organic Compounds in Exhaust Gas Samples.

Compound	**GB 06/01/2001 600 ^{o}C TOC < 1.0 P-1**	**H 06/04/2001 600 ^{o}C TOC < 1.0 P-5**	**GB 06/05/2001 550 ^{o}C TOC < 1.0 P-9**	**H 06/05/2001 550 ^{o}C TOC = 18 P-11**	**GB 06/06/2001 600 ^{o}C TOC < 1.0 P-13**	**H 06/06/2001 600 ^{o}C TOC < 1.0 P-16**
	Concentration, parts-per-billion (v/v)					
Chlorodifluoromethane	< 10	< 5.0	< 10	< 5.0	**42**	**49**
Propene	< 10	**83**	< 10	**4800**	< 10	**30**
Dichlorodifluromethane	< 10	< 10	< 10	< 10	< 10	< 10
Chloromethane	< 10	< 10	< 10	**320**	< 10	< 10
Dichlorotetrafluoroethane	< 10	< 10	< 10	< 10	< 10	< 10
Vinyl Chloride	< 10	**120**	< 10	**30**	< 10	< 10
1,3-Butadiene	< 10	< 10	< 10	**34**	< 10	< 10
Bromomethane	< 10	< 10	< 10	< 10	< 10	< 10
Chloroethane	< 10	< 10	< 10	**2200**	< 10	< 10
Acetonitrile	**67**	**53**	**50**	**100**	**47**	**81**
Acrolein	< 10	< 10	< 10	**22**	< 10	< 10
Acetone	**86**	**60**	**38**	**420**	**29**	**120**
Trichlorofluoromethane (R11)	< 10	< 10	< 10	< 10	< 10	< 10
Acrylonitrile	< 10	< 10	< 10	< 10	< 10	< 10
n-Pentane	< 10	< 10	< 10	**1500**	< 10	< 10
1,1 Dichloroethane	< 10	< 10	< 10	< 10	< 10	< 10
Methylene Chloride	< 10	< 10	< 10	**12**	< 10	< 10
3-Chloro-1-Propene	< 10	< 10	< 10	< 10	< 10	< 10
1,1,2-Trichlorotrifluoroethane	< 10	< 10	< 10	< 10	< 10	< 10
Carbon Disulfide	< 10	< 10	**17**	**28**	< 10	**11**
Trans-1,2-Dichloroethane	< 10	< 10	< 10	< 10	< 10	< 10
1,1, Dichloroethane	< 10	< 10	< 10	< 10	< 10	< 10
Vinyl Acetate	< 10	< 10	< 10	< 10	< 10	< 10
2-Butanone	< 10	< 10	< 10	**130**	< 10	< 10
Cis-1,2 Dichloroethene	< 10	< 10	< 10	< 10	< 10	< 10

Compound	GB 06/01/2001 600 °C TOC < 1.0 P-1	H 06/04/2001 600 °C TOC < 1.0 P-5	GB 06/05/2001 550 °C TOC < 1.0 P-9	H 06/05/2001 550 °C TOC = 18 P-11	GB 06/06/2001 600 °C TOC < 1.0 P-13	H 06/06/2001 600 °C TOC < 1.0 P-16
	Concentration, parts-per-billion (v/v)					
Hexane	**39**	**25**	< 10	**430**	**12**	**46**
Chloroform	< 10	< 10	< 10	**110**	< 10	< 10
1,2 Dichloroethane	< 10	< 10	< 10	< 10	< 10	< 10
1,1,1 Trichloroethane	< 10	< 10	< 10	< 10	< 10	< 10
Benzene	< 10	< 10	**86**	**470**	< 10	< 10
Carbon Tetrachloride	< 10	< 10	< 10	< 10	< 10	< 10
1,2 Dichloropropane	< 10	< 10	< 10	< 10	< 10	< 10
Bromodichloromethane	< 10	< 10	< 10	< 10	< 10	< 10
Trichloroethene	< 10	< 10	< 10	< 10	< 10	< 10
Methyl Methacrylate	< 10	< 10	< 10	**17**	< 10	< 10
Heptane	< 10	< 10	< 10	**180**	< 10	< 10
4-methyl-2-pentanone	< 10	< 10	< 10	< 10	< 10	< 10
Cis-1,3-Dichloropropene	< 10	< 10	< 10	< 10	< 10	< 10
Trans-1,3-Dichloropropene	< 10	< 10	< 10	< 10	< 10	< 10
1,1,2 Trichloroethane	< 10	< 10	< 10	< 10	< 10	< 10
Toluene	< 10	< 10	< 10	**330**	< 10	< 10
2-Hexanone	< 10	< 10	< 10	< 10	< 10	< 10
Dibromochloromethane	< 10	< 10	< 10	< 10	< 10	< 10
1,2 Dibromoethane	< 10	< 10	< 10	< 10	< 10	< 10
Octane	< 10	< 10	< 10	**83**	< 10	< 10
Tetrachloroethene	< 10	< 10	< 10	< 10	< 10	< 10
Chlorobenzene	< 10	< 10	< 10	< 10	< 10	< 10
Ethylbenzene	< 10	< 10	< 10	**31**	< 10	< 10
m/p Xylene	< 10	< 10	< 10	**180**	< 10	< 10
Bromoform	< 10	< 10	< 10	< 10	< 10	< 10
Styrene	< 10	< 10	< 10	< 10	< 10	< 10
1,1,2,2-Tetrachloroethane	< 10	< 10	< 10	< 10	< 10	< 10
o-Xylene	< 10	< 10	< 10	**51**	< 10	< 10
1,3,5-Trimethylbenzene	< 10	< 10	< 10	**25**	< 10	< 10
Alpha-methyl styrene	< 10	< 10	< 10	< 10	< 10	< 10
1,2,4-Trimethylbenzene	< 10	< 10	< 10	**42**	< 10	< 10
Benzyl Chloride	< 10	< 10	< 10	< 10	< 10	< 10
1,3-Dichlorobenzene	< 10	< 10	< 10	< 10	< 10	< 10
1,4-Dichlorobenzene	< 10	< 10	< 10	< 10	< 10	< 10
1,2-Dichlorobenzene	< 10	< 10	< 10	< 10	< 10	< 10
1,2,4-Trichlorobenzene	< 10	< 10	< 10	< 10	< 10	< 10

Compound	GB 06/01/2001 600 °C TOC < 1.0 P-1	H 06/04/2001 600 °C TOC < 1.0 P-5	GB 06/05/2001 550 °C TOC < 1.0 P-9	H 06/05/2001 550 °C TOC = 18 P-11	GB 06/06/2001 600 °C TOC < 1.0 P-13	H 06/06/2001 600 °C TOC < 1.0 P-16
	Concentration, parts-per-billion (v/v)					
Hexachlorobutadiene	< 10	< 10	< 10	< 10	< 10	< 10

5.5.2 Liquid Residuals

The liquid sample volumes generated by the performance tests were very limited. To obtain as much analytical data as possible on the treated liquid residue, the samples were processed as shown in Table 5-9.

Table 5-9 Liquid Sample Analyses

Num.	Date	Simulant	Temp °C	Time (min)	Liquid TOC	Analyses Performed				
						VOC	DMMP/ DMSO	Semi-VOC	Metals	Anions
P-1	**6/01/01**	GB/MEA	600	60	< 1.0	Combined	N/A	Combined	Combined	Combined
P-2	**6/01/01**	GB/MEA	600	60	< 1.0		N/A			
P-5	**6/04/01**	H/MEA	600	60	3.14	Combined	Combined	Combined	Combined	Combined
P-6	**6/04/01**	H/MEA	600	60	< 1.0					
P-9	**6/05/01**	GB/MEA	600	60	< 1.0	Analyzed	Analyzed	N/A	N/A	N/A
P-10	**6/05/01**	H/MEA	550	60	18	Analyzed	Analyzed	N/A	N/A	N/A
P-13	**6/06/01**	GB/MEA	600	60	< 1.0	Combined w/ P-17	N/A	Combined w/ P-17	Combined w/ P-17	Combined w/ P-17
P-16	**6/06/01**	H/MEA	600	60	< 1.0	Combined w/ P-20	N/A	Combined w/ P-20	Combined w/ P-20	Combined w/ P-20
P-17	**6/07/01**	GB/MEA	600	60	1.91	Combined w/ P-13	N/A	Combined w/ P-13	Combined w/ P-13	Combined w/ P-13
P-18	**6/07/01**	GB/MEA	600	60	< 1.0	Analyzed	Analyzed	N/A	N/A	N/A
P-19	**6/07/01**	H/MEA	600	60	4.43	Analyzed	Analyzed	N/A	N/A	N/A
P-20	**6/07/01**	H/MEA	600	60	< 1.0	Combined w/ P-16	N/A	Combined w/ P-16	Combined w/ P-16	Combined w/ P-16

N/A – Not Analyzed

5.5.2.1 Volatile Organic Compounds

Volatile Organic Compounds were analyzed by EPA method 8260. Sixty compounds were analyzed with a detection limit of 100 micrograms-per-liter (ppb). The entire listing of compounds analyzed and detection limits is contained in the analytical report in Appendix 2.

Table 5-10 lists the two compounds that were detected, acetone and carbon disulfide. Both were detected in the blank analyses. Upon consideration of the sample dilutions used in the analyses, only two samples (P-1 and P-2 Composited and P-10) can be viewed with any certainty as possessing acetone concentrations above background levels of 1400 ppb. The carbon disulfide

concentrations in all of the samples remain above background levels of about 470 ppb, taking into account the blank values and sample dilutions.

Table 5-10 Detected Volatile Organic Compounds in Liquid Residue

Compound	Concentration, micrograms per Liter							
	GB P-1 & P-2 Composite 600 °C TOC <1.0	GB P-9 550 °C TOC <1.0	GB P-13&P-17 Composite 600 °C TOC @ 1.9	GB P-18 600 °C TOC <1.0	H P-5 & P-6 Composite 600 °C TOC @ 3	H P-10 550 °C TOC = 18	H P-19 600 °C TOC = 4.4	H P-16&P-20 Composite 600 °C TOC <1.0
Acetone	2600	1700	1100	1000	1900	5900	1700	1100
Carbon Disulfide	650	640	1000	650	700	850	770	1000

5.5.2.2 DMMP and DMSO

The liquid residue was analyzed for dimethyl methylphosphonate (DMMP) and dimethyl sulfoxide (DMSO) as indicative of Schedule 2 compounds per the Chemical Weapons Convention (CWC) treaty. Of particular concern was that the Batch-SCWO process effectively destroy these compounds. The samples were analyzed using SwRI's internally developed GC/MS protocols. In all cases, the liquid residual was below the detection limit of 20 ppb for DMMP and 1000 ppb for DMSO.

5.5.2.3 Semi-Volatile Organic Compound Analyses

Four of the composited samples (see Table 5-9) were analyzed for semi-volatile organic compounds utilizing EPA Method 8270. Due to the small sample volumes available for extraction (10 compared to several hundred milliliters as indicated by the EPA Method), the detection limits were higher than the 10 microgram per Liter value typically reported by SwRI. Detection limits ranged from 100 to 1700 ppb and are listed in Appendix 2. None of the compounds were found in the samples at concentrations above their respective detection limits.

5.5.2.4 Metal Analyses

Table 5-11 presents the metal analyses of the treated liquid residue samples utilizing EPA Method SW-846 6110B.

The reactor vessel was fabricated of Inconel™ 625 Stainless Steel. The formulation of Inconel™ 625 is: Ni (+Co) 62.59%, Mn 0.55%, Fe 6.85%, Si 0.35%, Cu 0.05%, Cr 20%, Al 0.15%, and Ti 2.2%. It is evidence of the corrosive environment within the SCWO reactor that the detectable metals include all of the constituents of Alloy 625.

It should be noted that it was recognized at the onset of the testing that corrosion would occur within the system and that the metals in the liquid residual were expected. Materials of construction and corrosion management testing/optimization were not objectives of this testing. A recommendation is to address these issues in a subsequent phase once the efficacy of the process is demonstrated.

Table 5-11 Metal Analyses Liquid Residue.

Element	GB P-1 & P-2 Composite 600 °C TOC <1.0	GB P-13 & P-17 Composite 600 °C TOC @ 1.9	H P-5 & P-6 Composite 600 °C TOC @ 3	H P-16 & P-20 Composite 600 °C TOC <1.0
	Concentration in milligrams-per-liter			
Aluminum	**3.86**	**2.52**	**9.46**	**7.90**
Antimony	<0.2	<0.2	0.980	<0.2
Arsenic	0.091	<0.05	0.153	0.302
Barium	<0.05	<0.05	<0.05	<0.05
Beryllium	<0.05	<0.05	<0.05	<0.05
Bismuth	0.269	0.153	0.469	1.37
Boron	6.55	4.98	5.76	9.57
Cadmium	<0.05	<0.05	0.280	0.336
Calcium	0.766	0.603	1.24	1.53
Chromium	**965**	**626**	**1583**	**3465**
Cobalt	**1.28**	**0.651**	**1.44**	**0.348**
Copper	**0.339**	**0.213**	**2.66**	**0.187**
Iron	**4.59**	**5.88**	**7.17**	**8.08**
Lanthanum	<0.05	<0.05	<0.05	<0.05
Lead	<0.1	<0.1	<0.1	<0.2
Lithium	<0.05	<0.05	<0.05	<0.05
Magnesium	<1	<1	<1	<2
Manganese	**0.084**	**0.106**	**<0.05**	**<0.05**
Molybdenum	461	280	675	1846
Nickel	**96.9**	**100**	**80.4**	**89.5**
Palladium	<0.75	<0.75	<0.75	<0.75
Phosphorus	2722	2382	568	50.9
Potassium	15.0	12.1	51.3	10.3
Selenium	<0.1	<0.1	<0.1	<0.1
Silicon	**20.7**	**11.4**	**11.3**	**7.65**
Silver	<0.05	<0.05	<0.05	<0.05
Sodium	7182	6916	23445	5375
Strontium	<0.05	<0.05	<0.05	<0.05
Sulfur	9062	7127	21029	1947
Thallium	<1	<1	<1	<1
Thorium	<0.5	<0.5	<0.5	<0.5
Tin	2.32	1.73	7.66	0.576
Titanium	**0.205**	**0.220**	**1.03**	**0.146**
Tungsten	2.95	2.74	8.04	3.33
Uranium	<2	<2	<2	<2
Vanadium	<0.1	<0.1	<0.1	<2
Yttrium	<0.05	<0.05	<0.05	<0.05
Zinc	<0.05	<0.05	0.062	0.122
Zirconium	0.109	<0.05	0.071	<0.05

Items in bold are constituents of Inconel™ 625

5.5.2.5 Anion Analyses

Selected liquid samples were also analyzed for anion concentrations using an ion chromatographic method. Results of these analyses are presented in Table 5-12.

Table 5-12 Anion Analyses of Liquid Residue

Compound	Concentration milligrams-per-Liter			
	GB P-1 & P-2 Composite 600 °C TOC <1.0	**GB P-13 & P-17 Composite 600 °C TOC @ 1.9**	**H P-5 & P-6 Composite 600 °C TOC @ 3**	**H P-16 & P-20 Composite 600 °C TOC <1.0**
Fluoride	29.9	31.5	48.3	< 5.0
Chloride	<5.0	<5.0	1846	3034
Nitrite-N	<5.0	<5.0	<5.0	< 5.0
Nitrate-N	<5.0	<5.0	106	181
Sulfate	25584	18704	56833	5588

5.5.3 Solids

There were no solids generated during the performance testing of the simulated neutralents.

5.6 Material Balance

A material balance was performed on the system to evaluate both destruction efficiency of the process and determine the fate of specific heteroatoms.

5.6.1 Destruction Efficiency

The destruction efficiency of the batch-SCWO system is determined based on the TOC analyses of the feed and any residuals. The initial TOC is determined by the analyses of the simulant and based on that, the total milligrams of TOC in the reactor are determined. The residuals include the gas that is collected during depressurization of the reactor and the liquid that is collected. The destruction efficiency is simply the difference between the initial and final quantity of TOC divided by the initial amount of TOC.

In all performance test cases at, the preferred operating condition of 600 ^{o}C, the residual organic carbon in the vapor was trace (microgram quantities) and does not impact the amount of residual carbon. In the case of the liquid residual, most of the TOC analyses were below the detection limit of 1.0 ppm. In those cases, the destruction calculation assumed that 1.0 ppm of TOC was present. Table 5-13 is a summary of the destruction efficiencies noted in the tests.

Table 5-13 Performance Tests

Num.	Date	Simulant	Temp °C	Hold time (min)	Residual Liquid TOC (ppm)	Initial Organic Carbon (mg)	Residual Organic Carbon (mg)	Organic Carbon Destruction (%)	Comments
P-1	**6/01/01**	GB/MEA	600	60	< 1.0	756.6	0.0305	99.996	
P-2	**6/01/01**	GB/MEA	600	60	< 1.0	774.3	0.0305	99.996	
P-5	**6/04/01**	H/MEA	600	60	3.14	736.3	0.0856	99.988	
P-6	**6/04/01**	H/MEA	600	60	< 1.0	718.6	0.0397	99.994	
P-9	**6/05/01**	GB/MEA	550	60	< 1.0	754.2	0.0289	99.996	Low temperature test
P-10	**6/05/01**	H/MEA	550	60	18	732.8	0.4361	99.940	Low temperature test
P-13	**6/06/01**	GB/MEA	600	60	< 1.0	758.0	0.0276	99.996	
P-16	**6/06/01**	H/MEA	600	60	< 1.0	708.0	0.0244	99.997	
P-17	**6/07/01**	GB/MEA	600	60	1.91	758.0	0.0546	99.993	
P-18	**6/07/01**	GB/MEA	600	60	< 1.0	758.0	0.0296	99.996	
P-19	**6/07/01**	H/MEA	600	60	4.43	708.0	0.0244	99.988	
P-20	**6/07/01**	H/MEA	600	60	< 1.0	708.0	0.0247	99.997	

6. Test Results & Discussion – CAIS

6.1 Performance

Figure 6-1 shows the pressure and temperature history of a test run (run P-3) that was conducted with a simulated CAIS vial with no peroxide in the vessel. The vial broke at about 280 °C. The escaping chloroform raised the vessel pressure to about 270 psi. Four other ampules on other tests failed in the range of 235 to 250 °C. Figure 6-2 shows the shards of glass that were removed from the vessel after the test. There was no obvious change to the chloroform.

Figure 6-1 T and P History for a Simulated CAIS Vial in Empty Reactor

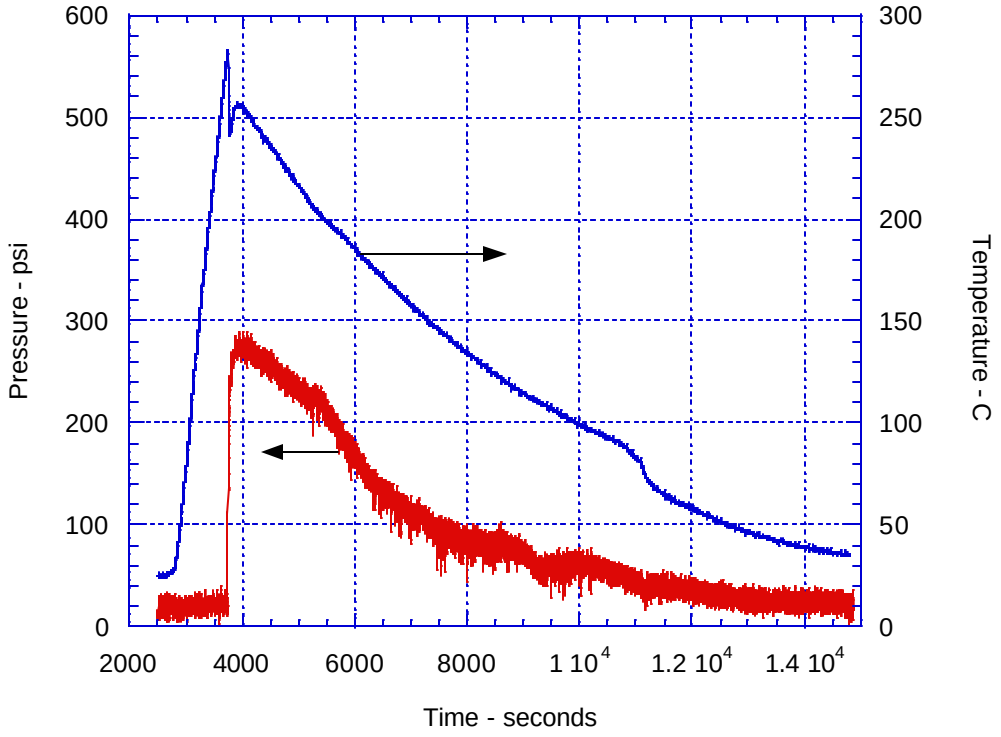


Figure 6-2 Glass Shards from CAIS Vial Burst in Empty Reactor

When the vessel contained hydrogen peroxide, the results were much different. Figure 6-3 and 6-4 show the pressure and temperature in the vessel, respectively. The initial spike at 3,300 seconds is from dissociation of the hydrogen peroxide as described earlier. The second spike at approximately 4,000 seconds occurred when the vial failed and the chloroform suddenly reacted with the hot oxidizer. Had there been more oxidant, there would have been more oxidation of the chloroform. However, the peak pressure and temperature would not change appreciably because there would also be more water in the vessel. Interestingly, the presence of the peroxide had no obvious effect on the temperature at which the ampules failed. During two tests with peroxide, the ampules broke at 240 and 256° C compared with 235 to 280 ^{o}C in the tests without peroxide.

The glass shards from this test, shown in Figure 6-6, were larger than on the test without hydrogen peroxide. The glass shards were a bright green due to corrosion products that were generated by the unneutralized chlorine that was generated in the presence of the oxygen from the peroxide.

Figure 6-3 Pressure History for a Simulated CAIS vial with Hydrogen Peroxide

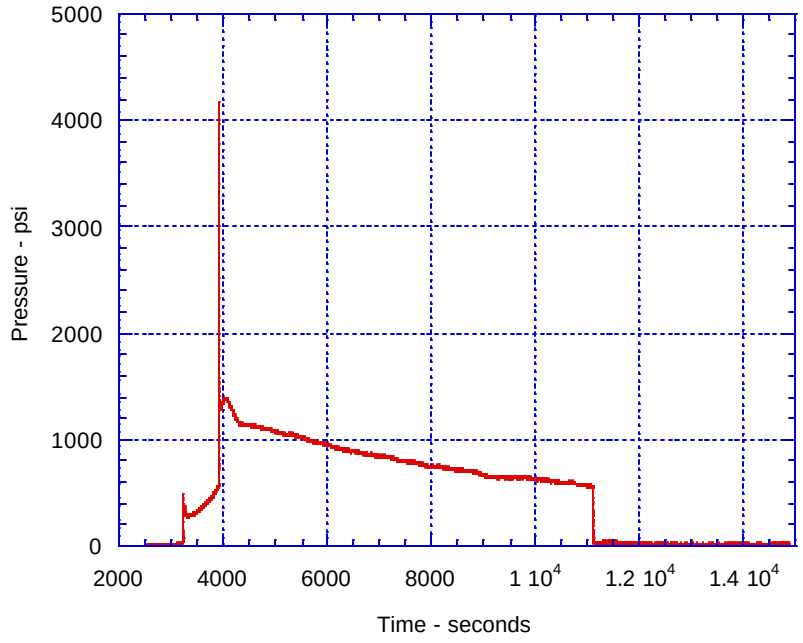


Figure 6-4Temperature History for a Simulated CAIS vial with Hydrogen Peroxide

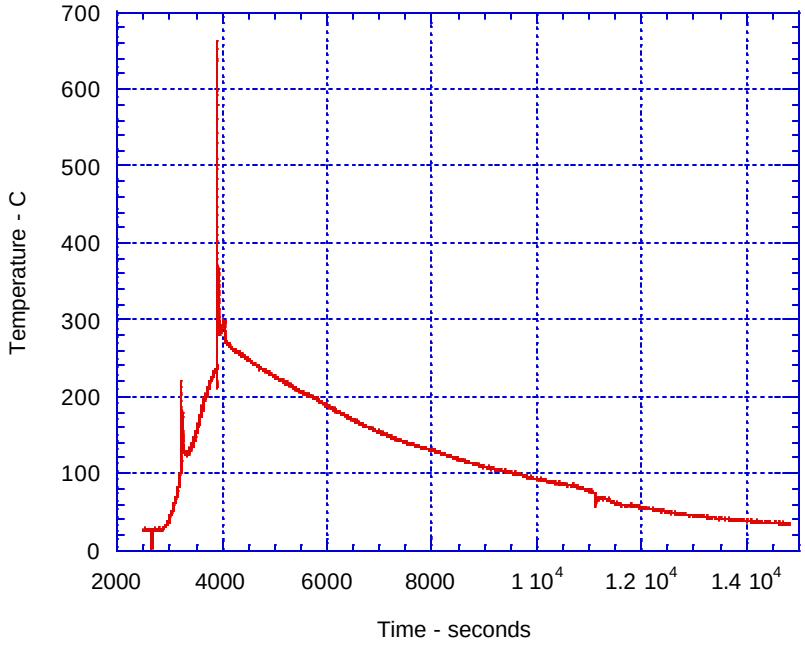


Figure 6-5 Glass Shards from Simulated CAIS Vial Tested with Hydrogen Peroxide

7. Applicability to NSCMP

Section 2 contains a discussion of the evolution of the batch-SCWO process within the NSCMP. Sandia initially presented it to the NSCMP in May 2000. The proposed application was a batch hydrothermal oxidation (BHO) system as an adjunct to the explosive destruction system (EDS) that was also under development by Sandia. The BHO process was viewed as a system that could accompany (or replace) the EDS and process the liquid neutralent that was generated during operations.

Stone & Webster was requested to conduct an evaluation of the BHO concept and recommended that the process focus on operations only at supercritical conditions (the original BHO operated at superheated subcritical conditions) hence the label of batch-SCWO. Stone & Webster also identified that the process was well suited to develop into a unit that could process individual CAIS vials or bottles. In fact, the fabrication of a unit capable of processing CAIS vials was a logical intermediate scale-up step in the process evolution.

7.1 Batch-SCWO Processing Concepts

Based on the results of this test program, Stone & Webster developed a concept for the scale-up and testing of the Batch-SCWO that included two scale-up steps resulting in a full-scale unit that was capable of processing live munitions with the capability to detonate and treat the agent in one vessel. The advantage of this system for the NSCMP is that the Batch-SCWO process offers a total solution in a single vessel unit that completely processes recovered CWM resulting in a clean residual that potentially could be disposed of in a simple manner.

The first step in the process development has been taken and was the demonstration of the process efficacy in treating the simulated neutralents and an ability to access CAIS vials within a sealed vessel.

The second step (Phase 2) would be the development and fabrication of a pilot system. Key to the development is fabricating a pilot system that is prototypical of full-scale operations including demonstrating the ability to detonate a simulated munition and process the residual at SCWO conditions. Stone & Webster recommends that the pilot system be based on a system sized to treat individual CAIS vials. This would require a vessel of approximately 5 to 6 gallons, which is adequate in size to demonstrate all aspects of full-scale operation in a prototypical manner. The pilot unit would be subjected to testing of simulated munitions to include the detonation of CWM as well as simulated CAIS.

Phase 3 of Batch-SCWO development is the fabrication and testing of a larger unit that would be capable of processing an entire munition of complete CAIS. The system would operate in a manner similar to the EDS in that the munition would be loaded and after the vessel is sealed; the munition would be detonated. The EDS process uses MEA-based neutralent to treat the agent contained in the munition. The resulting neutralent is still controlled under the Chemical Warfare Convention (CWC) Treaty and must be collected and processed prior to release. The metal parts must also be further treated to meet decontamination standards.

In addition to munitions, the full-size Batch-SCWO unit would be sized to be capable of processing a complete CAIS. This would involve applying a shape charge to the CAIS

container, loading it into the vessel and detonating the charges that would access the contents of the case. The Batch-SCWO vessel would then be heated and the material processed.

This full-sized Batch-SCWO process would be a vessel similar to the EDS, but fabricated with the additional design requirement to be capable of heating the vessel and contents to 600 ^{o}C allowing the agent materiel contained to be effectively destroyed. In fact, based on the operating conditions of 600 ^{o}C and residence times, the solid materials remaining would meet the 5X decontamination standards of time and temperature set by AR 385-61.

Based on the above approach, Stone & Webster conducted an analysis of the two processing concepts that make up the steps in scaling up the Batch-SCWO process (pilot and full-sized unit). The analysis was limited to evaluating the vessel design to identify any engineering issues that would limit the ability to fabricate or operate the process.

The specific areas addressed include:

- Projected Processing Vessel Size
- System Throughput
- Interface with Existing CAIS Recovery
- Corrosion Management
- Vessel Configuration
- Process/Equipment Operating Characteristics
- Reliability, Availability and Maintainability
- System Safety

7.2 Phase 2 - Pilot Unit

The processing vessel for the Phase 2 pilot scale Batch-SCWO process is sized based on the ability to process a simulated munition and single CAIS vial as an intermediate step to the full-sized unit. Note that the pilot unit is not intended as a production process for CAIS materiel, rather the intermediate scale-up step from the bench to full-size is approximately sized to accommodate a single CAIS vial. It is also convenient in that actual CWM may be processed through the use of existing CAIS vials.

CAIS materiels were developed and manufactured by the Department of the Army from the 1930's through the 1960's. Approximately 110,000 sets were manufactured. They were distributed for use by all services in training for identifying the various chemical agents that may be encountered on a battlefield.

In 1971, the Department of the Army declared the CAIS obsolete. In 1978 and 1980, two efforts were completed to gather and destroy existing CAIS that were not expended during training that were still in storage at various installations. More than 21,000 CAIS's were destroyed by December 1982, however, not all CAIS were accounted for. To date, some CAIS have been discovered at isolated storage locations. Periodically, CAIS continue to be found in this manner, and will need to be destroyed.[11]

Seventeen different sets of CAIS have been classified by both fill and configuration. One configuration, the K945 was completely destroyed. Table 7-1 is a summary of the various CAIS materiels that may be recovered [12].

The pilot-system developed for Phase 2 will be an intermediate size that is capable of processing simulated munitions and CAIS as well as individual CAIS vials/bottles as noted in Table 7-1. The unit will be capable of both accessing the contents through detonation and destroying the contents. In addition, the system will be assessed for its practicality in operation including evaluating normal operation, reliability and availability. In addition, the pilot testing will provide the engineering data to support the development of a conceptual design of the process.

Table 7-1 CAIS Materiels

Materiel		Agent (ml)	Chloroform (ml)	Charcoal (ml)
K 941 (3.5 ounce screw top bottles)				
	Sulfur Mustard	103	N/A	N/A
K 942 (3.8 ounce glass vial)				
	Sulfur Mustard	112	N/A	N/A
K 951/952 (80 ml glass vial)				
	Sulfur Mustard	2	38	N/A
	L {$C_2H_2AsCl_3$}	2	38	N/A
	PS {CCl_3NO_2}	20	20	N/A
	CG {CCl_2O}	40	N/A	N/A
K 953/954 (80 ml glass vial)				
	Sulfur Mustard	2	38	N/A
	HN {$(ClCH_2CH_2)_2NC_2H$}	4	36	N/A
	L {$C_2H_2AsCl_3$}	2	38	N/A
	CG {CCl_2O}	40	N/A	N/A
	CK {CClN}	40	N/A	N/A
	GA (simulant)	40	N/A	N/A
K 955 (3.5 ounce bottles w/ glass stoppers)				
	Sulfur Mustard	25	N/A	90
	L {$C_2H_2AsCl_3$}	25	N/A	90
	PS {CCl_3NO_2}	25	N/A	90
	CG (simulant)	6 grams	N/A	N/A
	CN {$C_6H_5COCH_2Cl$}	15 grams	N/A	N/A
	DM {$C_{12}H_9AsClN$}	15 grams	N/A	N/A

N/A – Not Analyzed

7.2.1 Processing Vessel Size

The potential CAIS materiel summarized in Table 7-1 were evaluated to determine the limiting case to set the design basis for the pilot unit vessel design. During processing the vessel is initially loaded with the reactants (CAIS vial, oxidant and caustic). As the heatup progresses, the waste associated with the hydrogen peroxide oxidant is vaporized. A 35% solution of hydrogen peroxide in water is used. The excess water serves to moderate the overall reaction, however it also is the major contributor to the system operating pressure. Higher pressures require thicker vessel walls, fabrication difficulty and increased cost.

Based on the organic loadings for the CAIS materiel listed in Table 7-1, it was determined that the K942 containing 3.8 ounces of Sulfur Mustard would require the most oxidant and associated water thereby generating the highest pressure at operating conditions.

Given that the system temperature is established at 600 ^{o}C to achieve destruction, the only remaining variable that can control system pressure is the vessel volume. Table 7-2 is a summary of the system pressure at several volumes. Based on the analyses, it was determined that a 5-gallon vessel should be used in order to limit system pressure to approximately 4000 psi. Note that the vessel sizing is based on a preliminary calculation and final vessel sizing will be conducted as a part of the Phase 2 activities.

Table 7-2 Processing Vessel Volume vs. Pressure for K942 Containing Neat Mustard

Reactor Volume	Pressure
3 gallon	6221 psi
4 gallon	4900 psi
5 gallon	4000 psi

For the feasibility analysis, a 7.75" ID x 24" long shell was assumed. The vessel wall and closure head thickness was determined from pressure design calculations performed in accordance with the ASME Boiler and Pressure Vessel Code, Section VIII, Division1. For a design pressure and temperature of 4000 psi and 1250 ^{o}F, assuming UNS N06617™ material, the vessel wall, lower head, and closure head thicknesses are 1.5", 2.5", and 4.75" respectively. The total weight of the vessel is estimated at 700 lbs.

7.2.2 System Throughput

The pilot unit is based on processing the equivalent loading of at least one CAIS vial in an eight-hour day. This is based on processing the limiting case of one K942 (3.8 ounce) mustard vial. When considering other CAIS, multiple vials/bottles may be processed based on the organic loading.

7.2.3 Corrosion Management

The Batch SCWO vessel design temperature and pressure is 4000 psi and 1250F with operating conditions between room temperature and design conditions for each batch cycle. A high temperature nickel base alloy is the best choice for these extreme conditions. Alloy UNS N06617™ is selected for the pressure-retaining boundary material.

The reactor vessel must be resistant to not only the mechanical aspects of the process (temperature, pressure and cyclic conditions) but also be resistant to the exposure conditions that will be present. Corrosion and metallurgical stability is therefore a significant concern. Of particular concern is the wide range in pH expected (less than 1 to 14) and the presence of chloride, fluoride, and acids (hydrofluoric and phosphoric acids).

Lead is also of concern. The glass material used in fabricating the vials and bottles may contain lead, which was added to increase the opacity of glass in their era of manufacture. Lead can cause embrittlement of steels resulting in premature and potentially catastrophic failure.

Testing is required to confirm the acceptability of this material – particularly in regards to the effect of fluoride and the type and amount of corrosion that would occur. Based on the service conditions noted above, there are no practical materials that will provide long term reliable service on exposure to these service conditions. Therefore all materials being considered should be considered as expendable. Consequently the best application would be as an expendable liner. The materials of choice for liner are:

1. Zirconium (Alloy 702)
2. Platinum
3. Tantalum
4. Titanium

Because of the lack of specific data on the behavior of these materials under these operating conditions, there are a number of uncertainties relating to their corrosion behavior. One unknown is the galvanic corrosion that may occur at mechanical connections between these materials and the pressure vessel. Another is the extent of oxidation (and resultant embrittlement) and the degradation that can occur from the alkali present. For each of these materials some limited testing should be performed to assess their behavior and life. In addition to the technical considerations availability and cost benefit studies should be performed to assess the economic advantages of each of these materials as expendable liners.

7.2.4 Vessel Configuration

The ASME Section VIII, Division 1, code-stamped pressure vessel is cylindrical in shape with a flat head and closure. A clamp type closure head is provided to facilitate removal during loading and unloading the vessel. For operational considerations, the vessel is oriented horizontally and skid mounted to facilitate future transportation. A tilting mechanism can be provided to facilitate the unloading of the vessel. A rupture disk will provide over-pressurization protection of the vessel. The emergency vent system shall be designed to ensure the complete containment of the reactor contents.

To minimize thermal discontinuities, handling and positioning provisions for the closure head and closure supports are not integral to the pressure boundary. For corrosion protection considerations a liner could be provided to insulate the pressure boundary material from the reaction products. Intermediate and final by-products of agent neutralization and SCWO destruction yield acids that are highly aggressive to nickel alloys. The liner is conceptualized as a thin (≈ 0.05”), close-fitting but non-integral member similar to cladding, extends over the closure surfaces. Final forming is obtainable by several methods including hydrostatic and Magnaform™.

Approximately four vessel penetrations would be required for instrumentation (pressure transducer, thermocouple, and pressure relief device) and sampling. From Phase I (bench) test results, these penetrations should be minimized and heated to reaction temperature in order to ensure complete reaction.

The pilot vessel will incorporate a fragment suppression system to mitigate the effects associated with explosive destruction of the simulated munition and CAIS. This system can be similar to that used in the Explosive Destruction System.

For the purpose of the feasibility analysis, electric ceramic fiber heating elements were used to heat the vessel. However, several alternatives will be evaluated during the design phase. Conceptually, the heaters would be supported in a space frame structure, which would stand off the vessel by 1" to 2". Preliminary calculations determined that with commercially available heaters the heatup time from ambient (21 ^{o}C) to 600 ^{o}C would take approximately 2 hours.

Cooldown would be accomplished by forced flow of ambient air through the annulus area between the heater face and the vessel (approximately 1 to 2 inches based on the manufacturer recommendations). At an air velocity of 50 feet-per-second the cooldown to 21 ^{o}C would take approximately 5 hours.

7.2.5 Process/Equipment Operating Characteristics

The pilot unit would follow the same basic operating steps as the bench-scale process:

- Load material and attach shape charges
- Install blast suppression shield
- Load reactants.
  - Oxidant (35 % hydrogen peroxide solution)
  - Caustic for neutralization (if required)
- Perform leak check
- Detonate material
- Heat the vessel to 600 ^{o}C
- Hold at temperature for one-hour
- Secure heaters and initiate cooling cycle
- Once vessel is cooled, sample TOC to verify destruction
- Once destruction is verified, open vessel and empty contents.

7.2.6 Reliability, Availability and Maintainability

The pilot Batch-SCWO vessel is subjected to temperature and pressure operating conditions that range between ambient and design conditions for each batch cycle. Since the vessel is heated externally by electric ceramic fiber heaters significant through wall thermal gradients will exist especially in regions of geometric discontinuities such as at the head to vessel intersection. The rate of heatup and cool-down of the vessel will thus affect the fatigue life and therefore both the rate and number of batch cycles that can be processed.

The feasibility analysis contained in Appendix 3 was performed to determine acceptable heatup and cool-down rates which could be achieved by conventional external heating methods, and to determine the fatigue life of the vessel due to thermal and pressure cycling.

The vessel response to thermal heatup and cool-down transients is calculated using the ANSYS™/Mechanical general-purpose finite element code. An axisymmetric model of the vessel shell, closure head, clamp and lower head is constructed using ANSYS™ PLANE55™ elements. The PLANE55™ is a 2-D thermal solid element that has thermal conduction capability for both steady-state and transient analyses.

The heatup transient is simulated by setting the initial model temperature to room temperature (70°F) and applying a heat flux to the outer surfaces of the model. A transient solution is then run and the resulting thermal gradients and end of transient temperatures reviewed. The heat flux and transient length is then adjusted and the model is rerun. Using an iterative procedure a reasonable heatup solution is determined. This solution is later confirmed to be acceptable by the fatigue analysis.

The cool-down transient is simulated by setting the model temperature at 1200°F and applying a forced air convection film coefficient and a bulk temperature of 70°F to the outer model surface. A transient solution is performed until the model approaches room temperature.

To determine vessel stresses due to both internal pressure and thermal gradient loads the ANSYS™ model is converted to PLANE42™ axisymmetric 2-D structural solid elements. Internal pressure is applied to the inner surfaces of the model and the resulting stress distribution is calculated. For thermal stress calculations the nodal temperature distribution from selected heatup and cool-down time steps is applied and a stress solution obtained.

To determine vessel fatigue life a design fatigue curve is developed in accordance with ASME Boiler and Vessel Code, Article III-2000 using vendor supplied fatigue test data. This was necessary since no design fatigue is available for the vessel alloy at the operating temperatures required. Using the ANSYS™ finite element results for the heatup, cool-down, and pressure cases the resulting stress range is calculated and the allowable number of operational cycles is determined from the design fatigue curve.

Table 7-3 summarizes the results of the pilot Batch SCWO vessel feasibility analysis. The heatup and cooldown rates will support processing of one operational cycle in a 24 hour period using external ceramic fiber heaters for heatup and forced convection for cool down. Fatigue life exceeds 2 years based on one cycle per day, 5 days a week operational period. It is concluded that the batch CAIS vial size SCWO vessel design is feasible for the intended use and does not require significant technology or fabrication process development for implementation.

7.2.7 System Safety

The Batch-SCWO pilot unit will operate at high temperatures and pressures. Safety, particularly personnel protection from hot surfaces and compressible fluids must be considered in the design. Numerous autoclaves are in existence that operate at similar conditions. Engineered safeguards including insulation and shielding to limit access to equipment and protect against failures.

A rupture disk will provide against over-pressurization of the vessel. Note that the rupture disk may require protection during the detonation. The rupture disk/emergency vent system will be designed to ensure the complete containment of the reactor contents.

The Batch-SCWO pilot vessel will incorporate a fragment suppression system to mitigate the effects associated with explosive destruction of the test materials. This system will be based on the design used in the Explosive Destruction System vessel.

Table 7-3 Phase 2 Processing Vessel Characteristics

Design Conditions:	Pressure	4000 psi
	Temperature	1250 F
Vessel Description:	Capacity	5 Gallon (19L)
Cylindrical Shape with a Flat Head and Closure	Material	UNS N06617™ Ni-Cr-Co-Mo Alloy
	Corrosion Barrier	Zirconium (Alloy 702)
	Shell	7.75" ID
	Shell Length	24"
	Shell Wall Thickness	1.5"
	Lower Head	2.5" thick
	Closure	REFLANGE G-CON 4.75" thick
Weight:	Closure	150 lbs.
	Clamp	140 lbs.
	Shell	320 lbs.
	Bottom Head	90 lbs.
	Total	700 lbs.
SCWO Heatup:	Power Input	7 to 20 watts/sq. in, 10 kW Total
Ceramic Fiber Heating Elements	Heatup Time	2 Hours
SCWO Cooldown:	Air Velocity	50 to 60 ft/sec
Forced Convection By Air	Cooldown Time	5 Hours
Fatigue Life:	Stress Range	95 ksi
	Allowable Cycles	1,600

7.3 Phase 3 – Munition/CAIS Processing Size

The processing vessel for the Phase 3 full scale Batch-SCWO process is sized based on the ability to process a single 4.2 inch mortar or intact CAIS. This concept basis was selected considering the inventory of recovered CWM that is contained at Pine Bluff Arsenal. The 4.2-inch mortars are the most numerous, representing 60 % of the inventory.

The full-scale concept being considered is a unit modeled after the existing Explosive Destruction System (EDS) that was developed by Sandia. The system would operate in a manner similar to the EDS in that the material would be loaded and the vessel sealed, and the munition or CAIS would be detonated.

This Batch-SCWO process would be a vessel similar to the EDS, but fabricated with the additional design requirement to be capable of heating the vessel and contents to 600 ^{o}C allowing the agent materiel to be effectively destroyed. In fact, based on the operating conditions of 600 ^{o}C and residence times, the solid materials remaining would meet the 5X decontamination standards of time and temperature.[13]

The system developed for Phase 3 will be capable of processing actual full-sized munitions and CAIS. The base case being a 4.2-inch mortar filled with sulfur mustard. Note that this analysis was limited to evaluation of the Batch-SCWO vessel to determine if the processing concept was feasible prior to commencing a development program.

7.3.1 Processing Vessel Size

The CWM inventory at Pine Bluff Arsenal was evaluated to determine the most prevalent item that could be the limiting case to set the design basis for the full-sized vessel design. As with the EDS, the vessel would be loaded with the munition in a detonation shield. Shape charges would be attached and electrically connected. In addition, the reactants (hydrogen peroxide solution and caustic) would also be added. The vessel is then sealed and leak checked. The munition then would be detonated and the heaters energized to begin system heatup. As the heatup progresses, the water associated with the hydrogen peroxide oxidant would be vaporized. A 35% solution of hydrogen peroxide in water is used. The excess water serves to moderate the overall reaction, however it also would be the major contributor to the system operating pressure.

The concept basis assumed a loading of mustard in the mortar of 6.25 pounds. The operating conditions of 600 ^{o}C, would provide complete destruction of the agent, and based on the reaction chemistry and system volume, the pressure can be determined. Table 7-4 is a summary of the system pressure at several volumes. Based on the analyses, it was determined that a 106-gallon (400 liter) vessel should be used in order to limit system pressure to approximately 4000 psi.

Table 7-4 Processing Vessel Volume vs. Pressure for 4.2 inch Mortar Containing Neat Mustard

Reactor Volume	Pressure
106 gallons	4000 psi
81 gallons	5000 psi
63.5 gallons	6000 psi

In order to minimize the design pressure requirements and resultant wall thickness, the largest size (106 gallon) vessel capacity was chosen. The ID was selected to match that of the EDS-1 design to accommodate the same blast suppression internals. The previous blast analyses stress calculations would also be applicable[14]. The resulting shell size is, therefore 20" ID x 78" long. Vessel wall and closure head thickness are determined from pressure design calculations performed in accordance with the ASME Boiler and Pressure Vessel Code, Section VIII, Division 1. For a design pressure and temperature of 4000 psi and 1250 ^{o}F, assuming UNS

N06617™ material, the vessel wall, lower head, and closure head thicknesses are 3.875", 6.375" and 8", respectively. The total weight of the vessel is estimated to be 11,500 lbs.

7.3.2 System Throughput

The initial goal was to be able to process one 4.2-inch mortar in an eight-hour day. However, as discussed in Section 7.3.6, the heatup and cooldown rates will not support that level of throughput, and it is more realistic to assume a throughput of one munition over a 24-hour day.

7.3.3 Interface with Existing Munition Recovery

At this time, it is assumed that the munition could be processed in the same manner as the EDS - that is the munition can be received without a secondary containment.

7.3.4 Vessel Configuration

While this would be based in large part on the lessons learned from the pilot unit, the processing concept evaluated by Stone & Webster is the same for the full-sized unit as the pilot. No scale-up problems related to the vessel configuration and closure mechanism are anticipated.

7.3.5 Corrosion Management

Corrosion management is still a particular concern. This concept analysis assumed that a lined vessel would be used based on the results of the pilot testing.

7.3.6 Process/Equipment Operating Characteristics

The full-sized unit would follow the same basic operating steps as the pilot-scale process with the exception of the detonation of the munition:

- Load material and attach shape charges
- Install blast suppression shield
- Load reactants.
  - Oxidant (35 % hydrogen peroxide solution)
  - Caustic for neutralization (if required)
- Perform leak check
- Detonate material
- Heat the vessel to 600 ^{o}C
- Hold at temperature for one-hour
- Secure heaters and initiate cooling cycle
- Once vessel is cooled, sample TOC to verify destruction
- Once destruction is verified, open vessel and empty contents

The method of heating of the vessels was chosen to be electric ceramic fiber heating elements. Preliminary calculations determined that with commercially available heaters the heatup time from ambient (21 ^{o}C) to 600 ^{o}C would take approximately 5 hours.

Cooldown would be accomplished by forced flow of ambient air through the annulus area between the heater face and the vessel (approximately 1 to 2 inches based on the manufacturer recommendations). At an air velocity of 50 feet-per-second the cooldown to 21 ^{o}C would take approximately 13 hours.

7.3.7 Reliability, Availability and Maintainability

The Munition Processing Batch SCWO vessel was analyzed using the same approach as was used for the CAIS vial size vessel and is described in Section 7.2. The detailed feasibility analysis is contained in the calculation included in Appendix 3. The results of the analysis are summarized in the Table 7-5.

The heatup and cooldown rates will support processing of one operational cycle in a 24 hour period using external ceramic fiber heaters for heatup and forced convection for cool down. Fatigue life exceeds 2 years based on one cycle per day, 5 days a week operational period. It is concluded that the full-size Batch-SCWO vessel design is feasible for the intended use and does not require significant technology or fabrication process development for implementation.

Table 7-5 Phase 2 Processing Vessel Characteristics

Design Conditions:	Pressure	4000 psi
	Temperature	1250 F
Vessel Description: *Cylindrical Shape with a Flat Head and Closure*	Capacity	106 Gallon (400L)
	Material	UNS N06617™ Ni-Cr-Co-Mo Alloy
	Corrosion Barrier	Zirconium (Alloy 702)
	Shell	20.00” ID
	Shell Length	78”
	Shell Wall Thickness	3.875”
	Lower Head	6.375” thick
	Closure	REFLANGE G-CON 8.00” thick
Weight:	Closure	1750 lbs.
	Clamp	1500 lbs.
	Shell	7000 lbs.
	Bottom Head	11500 lbs.
	Total	700 lbs.
SCWO Heatup: *Ceramic Fiber Heating Elements*	Power Input	7 to 15 watts/sq. in, 70 kW Total
	Heatup Time	5 Hours
SCWO Cooldown: *Forced Convection*	Air Velocity	50 to 60 ft/sec
	Cooldown Time	13Hours
Fatigue Life:	Stress Range	110 ksi
	Allowable Cycles	700

7.3.8 System Safety

The Phase 3 munition processing size Batch-SCWO vessel is to be designed and fabricated in accordance with the ASME Boiler and Pressure Vessel Code, Section V111, Division 1 to withstand 4000 psi internal design pressure at a design temperature of 1250 ^{o}F. For corrosion protection a Zr-702 liner is provided to insulate the pressure boundary material from reaction products. A rupture disk will provide against over-pressurization of the vessel. Note that the rupture disk may require protection during the detonation. The rupture disk/emergency vent system will be designed to ensure the complete containment of the reactor contents.

The Batch-SCWO vessel will incorporate a fragment suppression system to mitigate the effects associated with explosive destruction of the munition. This system can be identical to that used in the Explosive Destruction System Phase 1 vessel since the internal diameters of the EDS and Batch-SCWO vessels are the same. Since the Batch-SCWO vessel is significantly more robust than the EDS vessel, and its interior volume is greater, the Batch-SCWO vessel is more capable of withstanding the dynamic pressure loading associated with munition explosive destruction.

8. Conclusions

Test data and observations from the test runs completed of the Engineering Design Study Testing of the Batch-SCWO process were evaluated in accordance with the test criteria as described in Section 1. Test conclusions based on these criteria are summarized below.

- Nine out of ten tests at 600 ^{o}C demonstrated a destruction efficiency, based on TOC, of greater than 99.99 % for simulated GB and H neutralents. One test that did not make this target achieved a destruction efficiency of 99.988%.
- All tests at 600 ^{o}C demonstrated the ability of Batch-SCWO to process simulated GB and H neutralents and achieve a residual liquid TOC of less than 5 ppm. In 8 of the ten tests, the TOC was below the detection limit of 1.0 ppm.
- The Batch-SCWO process demonstrated a repeated and consistent ability to burst simulated K952 CAIS vials in the enclosed process during heatup.
- The liquid residuals from the process contained various concentrations of metals attributed to corrosion of the reactor vessel indicating that materials of construction and corrosion management need to be addressed through additional study in subsequent phases.
- The vapor residual from the tests at 600 ^{o}C, contained trace amounts (tens of parts-per-billion) of several volatile organic compounds, but none were at a level to pose a problem with permitting a system.
- The bench-scale system had several equipment-related problems (valve leakage and cold spots in instrumentation), that can be eliminated in subsequent designs.
- Based on the test results, preliminary concepts were developed for a two-step scale up of the process. The pilot-scale system is a 5 to 6 gallon vessel to demonstrate the ability to process simulated munitions as well as simulated CAIS and CAIS materiel. The full-scale system is a 106-gallon vessel that could process whole munitions and intact CAIS.
- Stress analyses of the conceptual processing vessels for the scale-up steps were completed to evaluate the Batch-SCWO operating concept's practicality in fabrication and operation. The process, as conceptualized, did not exceed allowable stresses and is feasible for the intended use.

9. Recommendations

- It is recommended that the Batch-SCWO process development proceed to the next level (Phase 2), which is the fabrication and testing of a 5 to 6 gallon pilot-scale unit capable of processing:
  - Simulated munitions
  - Simulated CAIS and actual CAIS components.
- A rigorous material of construction and corrosion management testing and evaluation program should be initiated to identify appropriate materials of construction and provide a quantitative indication of the reliability of the materials for pilot and full-scale operation.

10. References

[1] U.S. Army Project Manager for Non-Stockpile Chemical Materiel, Overarching Research Plan Non-Stockpile Chemical Materiel Program, June 9, 1999.

[2] Southwest Research Institute, H In MEA Simulant Preparation Procedure Version 1.1, April 24, 2001.

[3] Southwest Research Institute, GB In MEA Simulant Preparation Procedure Version 1.1, April 24, 2001.

[4] Drawing number A18-21-3 Miscellaneous Set, Gas Identification, Detonation Tube, Glass, August 2, 1932, revised June 30, 1955. Provided by NSCMP from archives.

[5] Sandia National Laboratories, Engineering Design Study of the Batch-SCWO Process to Treat Chemical Warfare Materiel, August 4, 2001

[6] Southwest Research Institute, H In MEA Simulant Preparation Procedure Version 1.1, April 24, 2001.

[7] Southwest Research Institute, GB In MEA Simulant Preparation Procedure Version 1.1, April 24, 2001.

[8] Southwest Research Institute, Analytical Report: Work-up and Performance Tests Sandia Batch SCWO Process – Final Report, September 13, 2001.

[9] Telephone communication between Jim Scott of Southwest Research Institute and Jeff Bettinger of Stone & Webster, September 25, 2001.

[10] Southwest Research Institute, Analytical Report: Work-up and Performance Tests Sandia Batch SCWO Process – Final Report, September 13, 2001.

[11] Rapid Response System Treatment Permit – Final, December 22, 1998

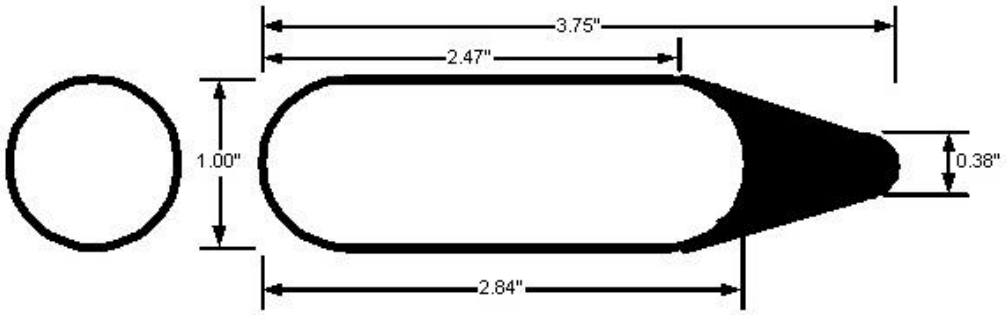
[12] U.S. Army Program Manager for Chemical Demilitarization, Chemical Agent Identification Sets (CAIS) Information Package, November 1995

[13] Department of the Army, Toxic Chemical Agent Safety Standards, Pamphlet 385-61, March 31, 1997

[14] U.S. Army Program Manager for Chemical Demilitarization - Product Manager for Non-Stockpile Chemical Materiel, Explosive Destruction System Phase 1 Interim Test Report, December 20, 2000.

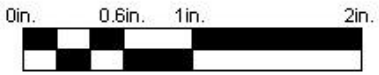
Appendix A

Simulated CAIS Vial Specification



Notes:

- All drawing dimensions shown are in inches
- Vial to be fabricated from Pyrex Glass
- Vial to be filled with 20 milliliters of pure Chloroform or other material as specified
- Tip of vial to be flame sealed
- Vial walls and bottom to be 1.5 mm thick glass



This half-height surrogate is based on the original dimensions and materials taken from *Chemical Agent Identification Sets Information Packge* by US Army PMCD, November 1995

REV.	DESCRIPTION	DATE	BY
O	Original Issue	3/29/01	JAB

Stone & Webster, Inc.

Simulated CAIS Vial - Half Size

SIZE	FSCM NO	DWG NO	REV
		1005537.400D	

SCALE	as shown	March 29, 2001	SHEET	1 OF 1

Appendix B

Analytical Report

Prepared by

Southwest Research Institute

Analytical Report:
Work-up and Performance Tests
Sandia Batch SCWO Process

Final Report

Contract Number: DAAM01-96-D-0010
Subcontract PS-028380 Delivery Order 37
SwRI Project: 01.03158.02

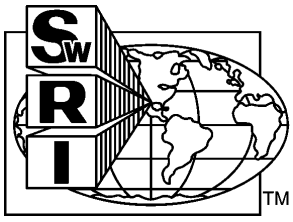
Prepared By

Jim Scott

Prepared For

Stone and Webster, Inc.
100 Technology Drive
Stoughton, MA 02072

September 13, 2001
(Revision 1.0 – October 1, 2001)



SOUTHWEST RESEARCH INSTITUTE
6220 Culebra Road · P.O. Drawer 28510
San Antonio, Texas 78228-0510

SOUTHWEST RESEARCH INSTITUTE
6220 CULEBRA ROAD • P.O. DRAWER 28510
SAN ANTONIO, TEXAS 78228-0510

Analytical Report: Work-up and Performance Tests Sandia Batch SCWO Process

Final Report

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Subcontract PS-028380 Delivery Order 37
SwRI Project: 01.03158.02

Prepared By

Jim Scott

Prepared For

Stone and Webster, Inc.
100 Technology Drive
Stoughton, MA 02072

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(Revision 1.0 – October 1, 2001)

APPROVED:

Michael G. MacNaughton, Ph.D., P.E.
Vice President
Chemistry and Chemical Engineering Division

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1. Introduction

Southwest Research Institute (SwRI) performed Professional Services for Sampling & Analysis to Support Engineering Design Study of the Batch SCWO Process to Treat NSCMP Neutralents and CAIS Materials under Stone and Webster Engineering Contract DAAM01-96-D-0010, Subcontract PS-028380, Delivery Order 37.

The samples were analyzed following the specifications contained within the Sampling and Analysis Plan (SAP) prepared by Stone and Webster dated 25 May 2001. Liquid and air samples were received from both the work-up and the performance testing phases. The work-up liquid samples were only analyzed for their Total Organic Carbon (TOC) content per instructions received from the Stone and Webster Project Officer. The volumes of the air samples from the work-up tests were too small to accomplish the complete array of analyses specified in the SAP, so as many analyses as possible to characterize the chemical quality of the SCWO gaseous effluent were performed.

Similarly, the volumes of the liquid samples generated by the performance tests were quite limited, approximately 19 to 30 milliliters (mLs). SwRI coordinated with the Stone and Webster Project Officer to obtain as much data as possible from these samples to characterize the organic and inorganic constituents of the treated liquid effluents.

The analytical data from the work-up and performance tests are summarized in the following sections. The sample analysis data sheets are also included in the Appendices as reference.

2. Total Organic Carbon Analyses

2.1 Work-Up Test Samples

SwRI received two batches of work-up test samples for analysis. The first batch consisted of 4 liquid samples all dated 30 April 2001, for TOC analysis. The samples were labeled as being from Vessels 1 through 4. Per instructions, the samples labeled Vessels 1 and 2 were combined for a composite TOC analysis, and similarly, the samples from Vessels 3 and 4 were combined for a composite analysis. The second batch of work-up samples consisted of 4 liquid samples for TOC analysis and Tedlar bags for air analysis. Table 1 presents the TOC data for the two batches of work-up samples.

2.2 Performance Test Samples

A total of 12 liquid samples were received, in two batches, and identified as performance test samples. The weights and volumes of the 12 samples as received were measured and the TOC analyses were performed. Subsequently, the liquid samples were composited utilizing instructions received from the Project officer for the remaining array of liquid analyses. Table 2 presents the TOC data for the 12 performance test samples. The TOC sample analysis data sheets for both the work-up and the performance tests are presented in Appendix A.

Table 1. TOC Analyses of Work-up Test Samples.

SwRI System ID	Sample Date	Sample Identifier	Total Organic Carbon, mg/L
160609	30 April 2001	Composite of Vessels 1 & 2	9.37 Duplicate: 8.25
160610	30 April 2001	Composite of Vessels 3 & 4	64.2
162383	14 May 2001	GB Vessel 1	5.17 Duplicate: 5.30
162384	21 May 2001	GB Vessel 1	< 1.0
162387	22 May 2001	H Vessel 3	< 1.0
162388	22 May 2001	H Vessel 4	< 1.0

Table 2. TOC Analyses of Performance Test Samples.

SwRI System ID	Sample Date	Sample Identifier	Weight Grams	Volume mLs	Total Organic Carbon mg/L
162385	01 June 2001	GB Vessel 1	30.53	29.6	< 1.0
162386	01 June 2001	GB Vessel 2	32.34	30.9	< 1.0
162389	04 June 2001	H Vessel 1	27.26	25.6	3.14
162390	04 June 2001	H Vessel 2	39.66	36.8	< 1.0
162641	05 June 2001	GB Vessel 1	28.89	29.1	< 1.0 Duplicate: < 1.0
162642	06 June 2001	GB Vessel 1	27.57	27.7	< 1.0
162643	07 June 2001	GB Vessel 1	28.58	28.8	1.91
162644	07 June 2001	GB Vessel 2	29.63	30.3	< 1.0
162645	05 June 2001	H Vessel 3	24.23	24.4	18.0
162647	06 June 2001	H Vessel 4	24.35	24.5	< 1.0
162646	07 June 2001	H Vessel 3	24.66	24.4	4.43
162648	07 June 2001	H Vessel 4	18.67	18.9	< 1.0

3. Air Sample Analyses

3.1 Work-Up Test Samples

The volumes of the Tedlar air sample bags from the work-up samples were insufficient to perform the complete array of analyses for each test vessel. The analyses performed on the work-up test samples were as follows:

- GB Vessel 1, 14 May 2001, SwRI ID 163314: Volatile organic compounds (VOC) per EPA Method TO-14.

- GB Vessel 1, 21 May 2001, SwRI ID 163315: Permanent gases (PG, oxygen, nitrogen, carbon dioxide) and carbon monoxide.

- H Vessel 3, 22 May 2001: SwRI ID 20162236 for sulfur dioxide, SwRI ID Acid-1 for hydrogen chloride and sulfuric acid; SwRI ID 20106336 for nitric oxide and nitrogen dioxide; and SwRI ID 20161889 for chlorine.

- H Vessel 4, 22 May 2001: SwRI ID 163316 for PG, carbon monoxide, and VOC by EPA Method TO-14; and SwRI 163323 for semi-volatile organics by EPA Method 8270.

3.2 Performance Test Samples

The Tedlar air sample bags from the performance test samples were analyzed in accordance with written instructions provided to SwRI by the Project Officer. The analyses performed on the performance test samples were as follows:

- GB Vessel 1, 01 June 2001: SwRI ID 163320 for PG, carbon monoxide, and VOC by EPA Method TO-14; and SwRI 163326 for semi-volatile organics by EPA Method 8270.

- GB Vessel 2, 01 June 2001: SwRI ID Acid-4 for hydrogen fluoride; and SwRI ID 20106327 for nitric oxide and nitrogen dioxide.

- GB Vessel 1, 05 June 2001: SwRI ID 163321 for PG, carbon monoxide, and VOC by EPA Method TO-14.

- GB Vessel 1, 06 June 2001: SwRI ID 163322 for PG, carbon monoxide, and VOC by EPA Method TO-14; and SwRI 163327 for semi-volatile organics by EPA Method 8270.

- GB Vessel 1, 07 June 2001: SwRI ID Acid-5 for hydrogen fluoride; and SwRI ID 20106332 for nitric oxide and nitrogen dioxide.

- H Vessel 2, 04 June 2001: SwRI ID 20153791 for sulfur dioxide, SwRI ID Acid-2 for hydrogen chloride and sulfuric acid; SwRI ID 20106334 for nitric oxide and nitrogen dioxide; and SwRI ID 20161887 for chlorine.

- H Vessel 1, 04 June 2001: SwRI ID 163317 for PG, carbon monoxide, and VOC by EPA Method TO-14; and SwRI 163324 for semi-volatile organics by EPA Method 8270.

- H Vessel 3, 05 June 2001: SwRI ID 163318 for PG, carbon monoxide, and VOC by EPA Method TO-14.

- H Vessel 4, 06 June 2001: SwRI ID 163319 for PG, carbon monoxide, and VOC by EPA Method TO-14; and SwRI 163325 for semi-volatile organics by EPA Method 8270.

- H Vessel 4, 07 June 2001: SwRI ID 20162232 for sulfur dioxide, SwRI ID Acid-3 for hydrogen chloride and sulfuric acid; SwRI ID 20106329 for nitric oxide and nitrogen dioxide; and SwRI ID 20163812 for chlorine.

3.3 Permanent Gases and Carbon Monoxide in SCWO Exhaust

These analyses were performed in accordance with SwRI TAP 01-0405-013 (Rev1/Sep 00) on two analytical sequences by using a 5A Mol Sieve column in conjunction with a PDHID detector for the carbon monoxide. While for the remaining gases a TCD detector was used in conjunction with an Alltech CTRI column. Table 3 presents gas concentrations measured in the samples. For carbon monoxide, a detection limit of 100 ppmv was obtained and none of the samples contained this compound at this limit. In order to obtain the best possible accuracy, the standards as well as the samples were run in duplicate to assure reproducibility and the average was used to calculate the concentration.

Table 3. Permanent Gases and Carbon Monoxide in SCWO Exhaust.

SwRI ID	Client_ID	Carbon Dioxide Percent	Oxygen Percent	Nitrogen Percent	Carbon Monoxide ppmv
163315	GB Vessel 1, 21 May 2001	31.2	42.3	17.7	< 100
163320	GB Vessel 1, 01 June 2001	32.1	42.7	15.7	< 100
163321	GB Vessel 1, 05 June 2001	33.9	43.2	12.3	< 100
163322	GB Vessel 1, 06 June 2001	31.2	41.7	17.1	< 100
163316	H Vessel 4, 22 May 2001	29.4	45.2	16.0	< 100
163317	H Vessel 1, 04 June 2001	14.7	59.4	17.5	< 100
163318	H Vessel 3, 05 June 2001	35.8	37.8	15.1	< 100
163319	H Vessel 4, 06 June 2001	28.6	44.3	17.2	< 100
Note : Each concentration presented represents the average of two injections. ppmv = parts per million by volume					

3.4 Inorganic Gas Analyses

The analytical results of the gases collected in the Tedlar sample bags for various inorganic analytes are presented in Table 4. The analytes include: sulfur dioxide (SO_2), chlorine (Cl_2), nitric oxide (NO), nitrogen dioxide (NO_2), sulfuric acid (H_2SO_4), hydrogen chloride (HCl), and hydrogen fluoride (HF). The gases within the Tedlar samples bags were extracted through the appropriate filters, sorbent tubes, or impinger solutions as detailed in the Sampling and Analysis Plan. Dividing the chemical masses presented in Table 4 by the respective air volumes exhausted from the test vessels (recorded by Sandia personnel) will yield the gas concentrations for the analytes. With the exception of trace quantities of hydrogen chloride found in two of the samples, the masses of all the other analytes in the samples were below the reported detection limits. The analytical data sheets for these analyses are in Appendix B.

Table 4. Inorganic Gas Analyses.

Sample ID	SwRI ID	Mass of Compound Detected, micrograms						
		SO_2	Cl_2	NO	NO_2	H_2SO_4	HCl	HF
GB Vessel 2, 01 June 2001	Acid - 4	NA	NA	NA	NA	NA	NA	< 1.6
	20106327	NA	NA	< 1.3	< 1.3	NA	NA	NA
GB Vessel 1, 07 June 2001	Acid - 5	NA	NA	NA	NA	NA	NA	< 1.6
	20106332	NA	NA	< 1.3	< 1.3	NA	NA	NA
H Vessel 3, 22 May 2001	20162236	< 2.0	NA	NA	NA	NA	NA	NA
	Acid - 1	NA	NA	NA	NA	< 2.0	1.9	NA
	20106336	NA	NA	< 1.3	< 1.3	NA	NA	NA
	20161889	NA	< 5.8	NA	NA	NA	NA	NA
H Vessel 2, 04 June 2001	20153791	< 2.0	NA	NA	NA	NA	NA	NA
	Acid - 2	NA	NA	NA	NA	< 2.0	1.3	NA
	20106334	NA	NA	< 1.3	< 1.3	NA	NA	NA
	20161887	NA	< 5.2	NA	NA	NA	NA	NA
H Vessel 4, 07 June 2001	20162232	< 2.0	NA	NA	NA	NA	NA	NA
	Acid - 3	NA	NA	NA	NA	< 2.0	< 1.0	NA
	20106329	NA	NA	< 1.3	< 1.3	NA	NA	NA
	20163812	NA	< 6.5	NA	NA	NA	NA	NA

3.5 Gas Analyses for Semi-Volatile Organic Compounds

The gases collected in the Tedlar sample bags were extracted through a XAD-2 resin sorbent and analyzed for semi-volatile organic compounds utilizing EPA Method 8270. Table 5 presents the results of these analyses. Only two compounds, butylbenzylphthalate andbis(2-Ethylhexyl)phthalate, were found above their respective detection limit. The masses of these two compounds were nearly identical in all of the samples, including the blank XAD-2 resin. Phthalate compounds are common environmental contaminants associated with synthetic polymeric compounds. It is strongly suspected that the presence of these two compounds in the samples are related to the sample collection method (i.e., the materiel used in the fabrication of the Tedlar sample bags, or the Tygon tubing used to pass the gas sample from the bags to the XAD-2 sorbent tubes) and other miscellaneous sources of background contamination, rather than being actual constituents of the exhaust gases. The analytical data sheets are given in Appendix C.

Table 5. Semi-Volatile Organic Compounds in Exhaust Gas Samples.

	Mass of Compound, Micrograms					
	Blank XAD2	**GB Vessel 1 1 June**	**GB Vessel 1 6 June**	**H Vessel 4 22 May**	**H Vessel 1 4 June**	**H Vessel 4 6 June**
Compound	**163310**	**163326**	**163327**	**163323**	**163324**	**163325**
N-Nitrosodimethylamine	< 2	< 2	< 2	< 2	< 2	< 2
Pyridine	< 2	< 2	< 2	< 2	< 2	< 2
Aniline	< 1	< 1	< 1	< 1	< 1	< 1
Bis(2-Chloroethyl)Ether	< 1	< 1	< 1	< 1	< 1	< 1
Phenol	< 1	< 1	< 1	< 1	< 1	< 1
2-Chlorophenol	< 1	< 1	< 1	< 1	< 1	< 1
1,3 Dichlorobenzene	< 1	< 1	< 1	< 1	< 1	< 1
1,4 Dichlorobenzene	< 1	< 1	< 1	< 1	< 1	< 1
1,2 Dichlorobenzene	< 1	< 1	< 1	< 1	< 1	< 1
Benzyl alcohol	< 5	< 5	< 5	< 5	< 5	< 5
Bis (2-aChloroisopropyl)-Ether	< 1	< 1	< 1	< 1	< 1	< 1
2-methylphenol	< 1	< 1	< 1	< 1	< 1	< 1
Hexachloroethane	< 1	< 1	< 1	< 1	< 1	< 1
N-Nitrosodi-n-	< 2	< 2	< 2	< 2	< 2	< 2
3 & 4 methylphenol	< 2	< 2	< 2	< 2	< 2	< 2
Nitrobenzene	< 1	< 1	< 1	< 1	< 1	< 1
Isophorone	< 1	< 1	< 1	< 1	< 1	< 1
2-Nitrophenol	< 2	< 2	< 2	< 2	< 2	< 2
2,4 Dimethylphenol	< 2	< 2	< 2	< 2	< 2	< 2
Bis (2-Chloroethoxy)-Methane	< 2	< 2	< 2	< 2	< 2	< 2
2,4 Dichlorophenol	< 2	< 2	< 2	< 2	< 2	< 2
1,2,4 Trichlorobenzene	< 1	< 1	< 1	< 1	< 1	< 1
Napthalene	< 1	< 1	< 1	< 1	< 1	< 1
Benzoic Acic	< 5	< 5	< 5	< 5	< 5	< 5
4-Chloroaniline	< 2	< 2	< 2	< 2	< 2	< 2
2,6 Dichlorophenol	< 2	< 2	< 2	< 2	< 2	< 2
Hexachlorobutadiene	< 1	< 1	< 1	< 1	< 1	< 1
4-Chloro-3-methylpheno	< 2	< 2	< 2	< 2	< 2	< 2
2-Methylnaphthalene	< 1	< 1	< 1	< 1	< 1	< 1
Hexachlorocyclo-pentadiene	< 5	< 5	< 5	< 5	< 5	< 5
2,4,6 trichlorophenol	< 2	< 2	< 2	< 2	< 2	< 2

Table 5 (continued). Semi-Volatile Organic Compounds in Exhaust Gas Samples.

	Mass of Compound, Micrograms					
	Blank XAD2	**GB Vessel 1 1 June**	**GB Vessel 1 6 June**	**H Vessel 4 22 May**	**H Vessel 1 4 June**	**H Vessel 4 6 June**
Compound	**163310**	**163326**	**163327**	**163323**	**163324**	**163325**
2,4,6 trichlorophenol	< 2	< 2	< 2	< 2	< 2	< 2
2-Chloronapthalene	< 2	< 2	< 2	< 2	< 2	< 2
1-Chloronapthalene	< 2	< 2	< 2	< 2	< 2	< 2
2-Nitroaniline	< 2	< 2	< 2	< 2	< 2	< 2
Acenaphthylene	< 1	< 1	< 1	< 1	< 1	< 1
Dimethylphthalate	< 1	< 1	< 1	< 1	< 1	< 1
2,6 Dinitrotoluene	< 5	< 5	< 5	< 5	< 5	< 5
Acenaphthene	< 1	< 1	< 1	< 1	< 1	< 1
3-Nitroaniline	< 2	< 2	< 2	< 2	< 2	< 2
2,4 Dinitrophenol	< 10	< 10	< 10	< 10	< 10	< 10
Dibenzofuran	< 1	< 1	< 1	< 1	< 1	< 1
2,4 Dinitrotoluene	< 1	< 1	< 1	< 1	< 1	< 1
4-Nitrophenol	< 5	< 5	< 5	< 5	< 5	< 5
Fluorene	< 1	< 1	< 1	< 1	< 1	< 1
4-Chlorophenyl-	< 1	< 1	< 1	< 1	< 1	< 1
Diethylphthalate	< 1	< 1	< 1	< 1	< 1	< 1
4-Nitroaniline	< 2	< 2	< 2	< 2	< 2	< 2
4,6 Dinitro-2-	< 2	< 2	< 2	< 2	< 2	< 2
N-Nitrosodiphenylamine and Diphenylamine	< 4	< 4	< 4	< 4	< 4	< 4
1,2 Diphenylhydrazine (as Azobenzene)	< 5	< 5	< 5	< 5	< 5	< 5
4-Bromophenyl-	< 2	< 2	< 2	< 2	< 2	< 2
Hexachlorobenzene	< 1	< 1	< 1	< 1	< 1	< 1
Pentachlorophenol	< 1	< 1	< 1	< 1	< 1	< 1
Phenanthrene	< 1	< 1	< 1	< 1	< 1	< 1
Anthracene	< 1	< 1	< 1	< 1	< 1	< 1
Carbazole	< 1	< 1	< 1	< 1	< 1	< 1
Di-n-butylphthalate	< 1	< 1	< 1	< 1	< 1	< 1
Isodrin	< 5	< 5	< 5	< 5	< 5	< 5
Fluoranthene	< 1	< 1	< 1	< 1	< 1	< 1
Benzidine	< 2	< 2	< 2	< 2	< 2	< 2
Pyrene	< 1	< 1	< 1	< 1	< 1	< 1
Butylbenzylphthalate	**22**	**27**	**23**	**23**	**23**	**22**

Table 5 (continued). Semi-Volatile Organic Compounds in Exhaust Gas Samples.

	Mass of Compound, Micrograms					
	Blank XAD2	**GB Vessel 1 1 June**	**GB Vessel 1 6 June**	**H Vessel 4 22 May**	**H Vessel 1 4 June**	**H Vessel 4 6 June**
Compound	**163310**	**163326**	**163327**	**163323**	**163324**	**163325**
3,3' Dichlorobenzidine		< 5	< 5	< 5	< 5	< 5
Benzo[a]anthracene		< 1	< 1	< 1	< 1	< 1
Chrysene		< 1	< 1	< 1	< 1	< 1
Bis(2-Ethylhexyl)-Phthalate	**1**	**1**	**1**	**1**	**1**	**1**
Di-n-octylphthalate		< 2	< 2	< 2	< 2	< 2
Benzo[b]fluoroanthene		< 1	< 1	< 1	< 1	< 1
Benzo[k]fluoroanthene		< 1	< 1	< 1	< 1	< 1
Benzo[a]pyrene		< 1	< 1	< 1	< 1	< 1
Indeno[1,2,3-cd]pyrene		< 5	< 5	< 5	< 5	< 5
Dibenz[a,h]anthracene		< 5	< 5	< 5	< 5	< 5
Benzo[g,h,I]perylene		< 5	< 5	< 5	< 5	< 5

3.6 Gas Analyses for Volatile Organic Compounds

The gases collected in the Tedlar sample bags were analyzed for their VOC content using EPA Method TO-14. Table 6 presents the results of the analyses. Since a known aliquot volume of gas was directly injected from the sample bag into the GC/MS, the concentrations of the VOC compounds could be calculated and represent the concentrations in the original gas sample. The first 62 compounds presented in the table are target compounds specified by the EPA Method TO-14 that are positively identified by the method protocol. Trace quantities of acetone were detected in the blank (as annotated in the analytical data sheets in Appendix D); thus, the true acetone concentrations in the sample will be slightly lower than depicted in Table 6. In addition, tentatively identified compounds detected by the GC/MS scan at concentrations above the detection limit (10 parts per billion, ppb) are listed at the end of the table.

Table 6. Volatile Organic Compounds in Exhaust Gas Samples.

	Concentration, parts per billion (v/v)							
	GB Vessel 1 14 May	**GB Vessel 1** 01 June	**GB Vessel 1** 05 June	**GB Vessel 1** 06 June	**H Vessel 4** 22 May	**H Vessel 1** 04 June	**H Vessel 3** 05 June	**H Vessel 4** 06 June
Compound	**163314**	**163320**	**163321**	**163322**	**163316**	**163317**	**163318**	**163319**
Chlorodifluoromethane	< 5.0	< 10	< 10	**42**	< 5.0	< 5.0	< 5.0	**49**
Propene	**540**	< 10	< 10	< 10	**83**	**83**	**4800**	**30**
Dichlorodifluromethane	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Chloromethane	**12**	< 10	< 10	< 10	**26**	< 10	**320**	< 10
Dichlorotetrafluoroethane	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10

Table 6 (continued). Volatile Organic Compounds in Exhaust Gas Samples.

	Concentration, parts per billion (v/v)							
	GB Vessel 1 14 May	**GB Vessel 1** 01 June	**GB Vessel 1** 05 June	**GB Vessel 1** 06 June	**H Vessel 4** 22 May	**H Vessel 1** 04 June	**H Vessel 3** 05 June	**H Vessel 4** 06 June
Compound	**163314**	**163320**	**163321**	**163322**	**163316**	**163317**	**163318**	**163319**
Vinyl Chloride	< 5.0	< 10	< 10	< 10	< 10	**120**	**30**	< 10
1,3-Butadiene	< 5.0	< 10	< 10	< 10	< 10	< 10	**34**	< 10
Bromomethane	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Chloroethane	< 5.0	< 10	< 10	< 10	< 10	< 10	**2200**	< 10
Acetonitrile	**12**	**67**	**50**	**47**	**59**	**53**	**100**	**81**
Acrolein	**10**	< 10	< 10	< 10	< 10	< 10	**22**	< 10
Acetone	**69**	**86**	**38**	**29**	**80**	**60**	**420**	**120**
Trichlorofluoromethane	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Acrylonitrile	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
n-Pentane	**16**	< 10	< 10	< 10	< 10	< 10	**1500**	< 10
1,1 Dichloroethane	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Methylene Chloride	**6.8**	< 10	< 10	< 10	< 10	< 10	**12**	< 10
3-Chloro-1-Propene	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
1,1,2Trichlorotrifluoroethane	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Carbon Disulfide	**28**	< 10	**17**	< 10	< 10	< 10	**28**	**11**
Trans-1,2-Dichloroethane	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
1,1, Dichloroethane	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Vinyl Acetate	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
2-Butanone	< 5.0	< 10	< 10	< 10	< 10	< 10	**130**	< 10
Cis-1,2 Dichloroethene	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Hexane	**34**	**39**	< 10	**12**	**34**	**25**	**430**	**46**
Chloroform	< 5.0	< 10	< 10	< 10	< 10	< 10	**110**	< 10
1,2 Dichloroethane	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
1,1,1 Trichloroethane	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Benzene	**310**	< 10	**86**	< 10	**31**	< 10	**470**	< 10
Carbon Tetrachloride	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
1,2 Dichloropropane	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Bromodichloromethane	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Trichloroethene	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Methyl Methacrylate	< 5.0	< 10	< 10	< 10	< 10	< 10	**17**	< 10
Heptane	< 5.0	< 10	< 10	< 10	< 10	< 10	**180**	< 10
4-methyl-2-pentanone	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Cis-1,3-Dichloropropene	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10

Table 6 (continued). Volatile Organic Compounds in Exhaust Gas Samples.

	Concentration, parts per billion (v/v)							
	GB Vessel 1 14 May	**GB Vessel 1** 1 June	**GB Vessel 1** 5 June	**GB Vessel 1** 6 June	**H Vessel 4** 22 May	**H Vessel 1** 4 June	**H Vessel 3** 5 June	**H Vessel 4** 6 June
Compound	**163314**	**163320**	**163321**	**163322**	**163316**	**163317**	**163318**	**163319**
Trans-1,3-Dichloropropene	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
1,1,2 Trichloroethane	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Toluene	**32**	< 10	< 10	< 10	< 10	< 10	**330**	< 10
2-Hexanone	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Dibromochloromethane	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
1,2 Dibromoethane	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Octane	< 5.0	< 10	< 10	< 10	< 10	< 10	**83**	< 10
Tetrachloroethene	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Chlorobenzene	**8.0**	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Ethylbenzene	< 5.0	< 10	< 10	< 10	< 10	< 10	**31**	< 10
m/p Xylene	< 5.0	< 10	< 10	< 10	< 10	< 10	**180**	< 10
Bromoform	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Styrene	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
1,1,2,2-Tetrachloroethane	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
o-Xylene	< 5.0	< 10	< 10	< 10	< 10	< 10	**51**	< 10
1,3,5-Trimethylbenzene	< 5.0	< 10	< 10	< 10	< 10	< 10	**25**	< 10
Alpha-methyl styrene	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
1,2,4-Trimethylbenzene	< 5.0	< 10	< 10	< 10	< 10	< 10	**42**	< 10
Benzyl Chloride	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
1,3-Dichlorobenzene	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
1,4-Dichlorobenzene	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
1,2-Dichlorobenzene	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
1,2,4-Trichlorobenzene	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Hexachlorobutadiene	< 5.0	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Tentatively Identified Compounds (TICS)								
Acetaldehyde	**10**	< 10	< 10	< 10	**12**	**18**	< 10	< 10
1-Propene, 2-methyl	**24**	< 10	< 10	< 10	< 10	< 10	**181**	**49**
Isopropyl Alcohol	**110**	**19**	**140**	< 10	**42**	**26**	< 10	**49**
Benzene, Hexafluoro	**96**	< 10	< 10	**23**	< 10	< 10	< 10	< 10
Benzaldehyde	**13**	**19**	**31**	**28**	**20**	**22**	< 10	**20**
Octane, 4-Methyl	< 10	**11**	< 10	< 10	< 10	< 10	< 10	< 10
Propane	< 10	< 10	< 10	< 10	< 10	< 10	**460**	**47**
Isobutane	< 10	< 10	< 10	< 10	< 10	< 10	**340**	**21**

Table 6 (continued). Volatile Organic Compounds in Exhaust Gas Samples.

	Concentration, parts per billion (v/v)							
	GB Vessel 1 14 May	**GB Vessel 1** 1 June	**GB Vessel 1** 5 June	**GB Vessel 1** 6 June	**H Vessel 4** 22 May	**H Vessel 1** 4 June	**H Vessel 3** 5 June	**H Vessel 4** 6 June
Compound	**163314**	**163320**	**163321**	**163322**	**163316**	**163317**	**163318**	**163319**
Tentatively Identified Compounds (TICS)								
Butane	< 10	< 10	< 10	< 10	< 10	< 10	**130**	**18**
2-Methyl Butane	< 10	< 10	< 10	< 10	< 10	< 10	**290**	< 10
2-Methyl Pentane	< 10	< 10	< 10	< 10	< 10	< 10	**76**	< 10
3-Methyl Hexane	< 10	< 10	< 10	< 10	< 10	< 10	**79**	< 10
Methyl Cyclohexane	< 10	< 10	< 10	< 10	< 10	< 10	**60**	< 10
Nonane	< 10	< 10	< 10	< 10	< 10	< 10	**57**	< 10
N,N-Dimethyl Acetamide	< 10	< 10	< 10	< 10	< 10	< 10	< 10	**29**

4. Treated Liquid Residue Analyses

As seen in Table 2, the liquid sample volumes generated by the performance tests were very limited. To obtain as much analytical data on the treated liquid residue, the samples were processed as follows per the written instructions provided by the Project Officer:

- GB Vessels1 and 2 combined, 01 June 2001: VOC analyses and as many analyses as possible.
- GB Vessel 1, 05 June 2001: VOC analyses and DMMP.
- GB Vessel 2, 07 June 2001: VOC analyses and DMMP.
- GB Vessel 1, 06 June 2001, combined with GB Vessel 1, 07 June 2001: As many analyses as possible.
- H Vessels 1 and 2 combined, 04 June 2001: VOC and as many analyses as possible.
- H Vessel 3, 05 June 2001: VOC analyses and DMSO.

- H Vessel 3, 05 June 2001: VOC analyses and DMSO.

- H Vessel 3, 07 June 2001: VOC analyses and DMSO.
- H Vessel 4, 06 June 2001, combined with H Vessel 4, 07 June 2001: As many analyses as possible.

4.1 Volatile Organic Compound Analyses, DMMP, and DMSO

Table 7 presents the VOCs detected in the treated liquid residue samples utilizing EPA Method 8260. As discussed in the analytical data sheets (Appendix E), acetone and carbon disulfide were detected in the blank analyses. Upon consideration of the sample dilutions used in the analyses, only two samples (162377 and 162670) can be viewed with any certainty as possessing acetone concentrations above background levels (about 1400 ug/L). The carbon disulfide concentrations in all of the samples remain above background levels (about 470 ug/L) taking into account the blank values and sample dilutions. Finally, the DMMP and DMSO concentrations for several samples utilizing SwRI's internally developed GC/MS protocols are also presented in Table 7.

Table 7. Volatile Organic Compounds, DMMP, and DMSO in Treated Liquid Residue Samples.

	Concentration, micrograms per Liter (ug/L)							
	GB Vessels 1 and 2 combined 1 June	**GB Vessel 1 5 June**	**GB Vessel 1 combined 6 and 7 June**	**GB Vessel 2 7 June**	**H Vessels 1 and 2 combined 4 June**	**H Vessel 3 5 June**	**H Vessel 3 7 June**	**H Vessel 4 combined 6 and 7 June**
Compound	**162377**	**162665**	**162667**	**162668**	**162379**	**162669 & 162670**	**162671 & 162672**	**162674**
DMMP		< 20		< 20				
DMSO					< 1000	< 1000	< 1000	
Dichlorodi-fluromethane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Chloro-methane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Vinyl Chloride	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Bromo-methane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Chloroethane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Acetone	**2600**	1700	1100	1000	1900	**5900**	1700	1100
Trichloro-fluoromethane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Acrylonitrile	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,1 Dichloro-ethane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Methylene Chloride	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Carbon Disulfide	**650**	**640**	**1000**	**650**	**700**	**850**	**770**	**1000**
Trans-1,2-di-chloroethane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,1, Dichloro-ethane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
2-Butanone	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Cis-1,2 Di-chloroethene	< 500	< 500	< 500	< 500	< 500	< 500	< 500	< 500
Chloroform	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
2,2 Dichloro-propane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,2 Dichloro-ethane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,1,1 trichloro-ethane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100

Table 7 (continued). Volatile Organic Compounds, DMMP, and DMSO in Treated Liquid Residue Samples.

	Concentration, micrograms per Liter							
	GB Vessels 1 and 2 combined 1 June	GB Vessel 1 5 June	GB Vessel 1 combined 6 and 7 June	GB Vessel 2 7 June	H Vessels 1 and 2 combined 4 June	H Vessel 3 5 June	H Vessel 3 7 June	H Vessel 4 combined 6 and 7 June
Compound	162377	162665	162667	162668	162379	162669 & 162670	162671 & 162672	162674
Benzene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Carbon Tetrachloride	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Dibromo-methane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,2 Dichloro-propane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Bromodi-chloromethane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Trichloro-ethene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
4-methyl-2-pentanone	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Cis-1,3-Di-chloropropene	< 500	< 500	< 500	< 500	< 500	< 500	< 500	< 500
Trans-1,3-Di-chloropropene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,1,2 Tri-chloroethane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,3 Dichloro-propane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Toluene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
2-Hexanone	< 500	< 500	< 500	< 500	< 500	< 500	< 500	< 500
Dibromo-chloromethane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,2 Dibromo-ethane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Tetrachloro-ethene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,1,1,2-Tetra-chloroethane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Chlorobenzene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Ethylbenzene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
m/p Xylene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Bromoform	< 200	< 200	< 200	< 200	< 200	< 200	< 200	< 200
Styrene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,1,2,2-Tetra-chloroethane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
o-Xylene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,2,3 Tri-chloropropane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Isopropyl-benzene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100

Table 7 (continued). Volatile Organic Compounds, DMMP, and DMSO in Treated Liquid Residue Samples.

	Concentration, micrograms per Liter							
	GB Vessels 1 and 2 combined 1 June	GB Vessel 1 5 June	GB Vessel 1 combined 6 and 7 June	GB Vessel 2 7 June	H Vessels 1 and 2 combined 4 June	H Vessel 3 5 June	H Vessel 3 7 June	H Vessel 4 combined 6 and 7 June
Compound	162377	162665	162667	162668	162379	162669 & 162670	162671 & 162672	162674
Bromobenzene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
n-Propyl-benzene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
2-Chlorotoluene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
4-Chlorotoluene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,3,5-Tri-methylbenzene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,2,4-Tri-methylbenzene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Tert-butylbenzene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,3-Dichloro-benzene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,4-Dichloro-benzene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
Sec-butylbenzene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
p-Isopropyl-toluene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,2 Dichloro-benzene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
n-butylbenzene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,2dibromo-3-chloropropane	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100
1,2,4-Tri-chlorobenzene	< 100	< 100	< 100	< 100	< 100	< 100	< 100	< 100

4.2 Semi-Volatile Organic Compound Analyses

Table 8 presents the semi-volatile organic compound analyses of the treated liquid residue samples utilizing EPA Method 8270. Due to the small sample volumes available for extraction (10 mLs compared to several hundred mLs as indicated by the EPA Method), the detection limits are higher than the 10 microgram per Liter value typically reported by SwRI. None of the compounds were found in the samples at concentrations above their respective detection limits. The analytical data sheets are presented in Appendix F.

Table 8. Semi-Volatile Organic Compounds in Treated Liquid Residue Samples.

	Concentration, micrograms per Liter			
	GB Vessels 1 & 2 combined, 01 June	**GB Vessel 1, combined 06 & 07 June**	**H Vessels 1 & 2 combined, 04 June**	**H Vessel 4, combined 06 & 07 June**
Compound	**162377**	**162667**	**162379**	**162674**
N-Nitrosodimethylamine	< 200	< 200	< 200	< 690
Pyridine	< 200	< 200	< 200	< 690
Aniline	< 100	< 100	< 100	< 340
Bis(2-Chloroethyl)Ether	< 100	< 100	< 100	< 340
Phenol	< 100	< 100	< 100	< 340
2-Chlorophenol	< 100	< 100	< 100	< 340
1,3 Dichlorobenzene	< 100	< 100	< 100	< 340
1,4 Dichlorobenzene	< 100	< 100	< 100	< 340
1,2 Dichlorobenzene	< 100	< 100	< 100	< 340
Benzyl alcohol	< 500	< 500	< 500	< 1700
Bis(2-Chloroisopropyl)Ether	< 100	< 100	< 100	< 340
2-methylphenol	< 100	< 100	< 100	< 340
Hexachloroethane	< 100	< 100	< 100	< 340
N-Nitrosodi-n-Propylamine	< 200	< 200	< 200	< 690
3 & 4 methylphenol	< 200	< 200	< 200	< 690
Nitrobenzene	< 100	< 100	< 100	< 340
Isophorone	< 100	< 100	< 100	< 340
2-Nitrophenol	< 200	< 200	< 200	< 690
2,4 Dimethylphenol	< 200	< 200	< 200	< 690
Bis(2-chloroethoxy)methane	< 200	< 200	< 200	< 690
2,4 Dichlorophenol	< 200	< 200	< 200	< 690
1,2,4 Trichlorobenzene	< 100	< 100	< 100	< 340
Napthalene	< 100	< 100	< 100	< 340
Benzoic Acid	< 500	< 500	< 500	< 1700
4-Chloroaniline	< 200	< 200	< 200	< 690
2,6 Dichlorophenol	< 200	< 200	< 200	< 690
Hexachlorobutadiene	< 100	< 100	< 100	< 340
4-Chloro-3-methylpheno	< 200	< 200	< 200	< 690
2-Methylnaphthalene	< 100	< 100	< 100	< 340
Hexachlorocyclopentadien	< 500	< 500	< 500	< 1700
2,4,6 trichlorophenol	< 200	< 200	< 200	< 690
2,4,6 trichlorophenol	< 200	< 200	< 200	< 690
2-Chloronapthalene	< 200	< 200	< 200	< 690

Table 8 (continued). Semi-Volatile Organic Compounds in Treated Liquid Residue Samples.

	Concentration, micrograms per Liter			
	GB Vessels 1 & 2 combined, 01 June	**GB Vessel 1, combined 06 & 07 June**	**H Vessels 1 & 2 combined, 04 June**	**H Vessel 4, combined 06 & 07 June**
Compound	**162377**	**162667**	**162379**	**162674**
1-Chloronapthalene	< 200	< 200	< 200	< 690
2-Nitroaniline	< 200	< 200	< 200	< 690
Acenapththylene	< 100	< 100	< 100	< 340
Dimethylphthalate	< 100	< 100	< 100	< 340
2,6 Dinitrotoluene	< 500	< 500	< 500	< 1700
Acenaphthene	< 100	< 100	< 100	< 340
3-Nitroaniline	< 200	< 200	< 200	< 690
2,4 Dinitrophenol	< 100	< 100	< 100	< 340
Dibenzofuran	< 100	< 100	< 100	< 340
2,4 Dinitrotoluene	< 100	< 100	< 100	< 340
4-Nitrophenol	< 500	< 500	< 500	< 1700
Fluorene	< 100	< 100	< 100	< 340
4-Chlorophenyl-phenyethe	< 100	< 100	< 100	< 340
Diethylphthalate	< 100	< 100	< 100	< 340
4-Nitroaniline	< 200	< 200	< 200	< 690
4,6 Dinitro-2-methylpheno	< 200	< 200	< 200	< 690
N-Nitrosodiphenylamine and Diphenylamine	< 400	< 400	< 400	< 1400
1,2 Diphenylhydrazine (as Azobenzene)	< 500	< 500	< 500	< 1700
4-Bromophenyl-phenylethe	< 200	< 200	< 200	< 690
Hexachlorobenzene	< 100	< 100	< 100	< 340
Pentachlorophenol	< 100	< 100	< 100	< 340
Phenanthrene	< 100	< 100	< 100	< 340
Anthracene	< 100	< 100	< 100	< 340
Carbazole	< 100	< 100	< 100	< 340
Di-n-butylphthalate	< 100	< 100	< 100	< 340
Isodrin	< 500	< 500	< 500	< 1700
Fluoranthene	< 100	< 100	< 100	< 340
Benzidine	< 200	< 200	< 200	< 690
Pyrene	< 100	< 100	< 100	< 340
Butylbenzylphthalate	< 100	< 100	< 100	< 340
3,3' Dichlorobenzidine	< 500	< 500	< 500	< 1700

Table 8 (continued). Semi-Volatile Organic Compounds in Treated Liquid Residue Samples.

	Concentration, micrograms per Liter			
	GB Vessels 1 & 2 combined, 01 June	**GB Vessel 1, combined 06 & 07 June**	**H Vessels 1 & 2 combined, 04 June**	**H Vessel 4, combined 06 & 07 June**
Compound	**162377**	**162667**	**162379**	**162674**
Benzo[a]anthracene	< 100	< 100	< 100	< 340
Chrysene	< 100	< 100	< 100	< 340
Bis(2-Ethylhexyl)Phthalate	< 200	< 200	< 200	< 690
Di-n-octylphthalate	< 200	< 200	< 200	< 690
Benzo[b]fluoroanthene	< 100	< 100	< 100	< 340
Benzo[k]fluoroanthene	< 100	< 100	< 100	< 340
Benzo[a]pyrene	< 100	< 100	< 100	< 340
Indeno[1,2,3-cd]pyrene	< 500	< 500	< 500	< 1700
Dibenz[a,h]anthracene	< 500	< 500	< 500	<1700
Benzo[g,h,I]perylene	< 500	< 500	< 500	< 1700

4.3 Metal Analyses of Solid Residue and Treated Liquid Residue

Table 9 presents the metal analyses of the treated liquid residue samples utilizing EPA Method SW-846 6110B. In addition to the treated liquid residue analyses, a sample of solids labeled as "scale" was also analyzed for its metals content. The analytical data sheets for the metals are in Appendix G.

Table 9. Metal Analyses of Solid Residue and Treated Liquid Residue.

	Concentration, parts per million (mg/kg for solid, mg/L for liquids)						
	Solids ("scale")		GB Vessels 1 & 2 combined, 01 June		GB Vessel 1 combined from 06 and 07 June	H Vessels 1 & 2 combined, 04 June	H Vessel 4 combined from 06 and 07 June
	Original Analysis	Duplicate	Original Analysis	Duplicate			
Element	163313		162377		162667	162379	162674
Aluminum	588	562	3.86	3.87	2.52	9.46	7.90
Antimony	34.3	35.8	<0.2	<0.2	<0.2	0.980	<2
Arsenic	<2	<2	0.091	0.081	<0.05	0.153	0.302
Barium	<1	<1	<0.05	<0.05	<0.05	<0.05	<0.05
Beryllium	<10	<10	<0.05	<0.05	<0.05	<0.05	<0.05
Bismuth	15.4	15.9	0.269	0.289	0.153	0.469	1.37
Boron	21.7	12.1	6.55	6.59	4.98	5.76	9.57
Cadmium	<3	<3	<0.05	<0.05	<0.05	0.280	0.336
Calcium	24.8	23.1	0.766	0.764	0.603	1.24	1.53
Chromium	23289	23047	965	951	626	1583	3465
Cobalt	231	230	1.28	1.28	0.651	1.44	0.348
Copper	123	106	0.339	0.344	0.213	2.66	0.187
Iron	7802	7684	4.59	4.63	5.88	7.17	8.08

Table 9 (continued). Metal Analyses of Solid Residue and Treated Liquid Residue.

	Concentration, parts per million (mg/kg for solid, mg/L for liquids)						
	Solids ("scale")		GB Vessels 1 & 2 combined, 01 June		GB Vessel 1 combined from 06 and 07 June	H Vessels 1 & 2 combined, 04 June	H Vessel 4 combined from 06 and 07 June
	Original Analysis	Duplicate	Original Analysis	Duplicate			
Element	163313		162377		162667	162379	162674
Lanthanum	<5	<5	<0.05	<0.05	<0.05	<0.05	<0.05
Lead	<25	<25	<0.1	<0.1	<0.1	<0.1	<0.2
Lithium	<1	<1	<0.05	<0.05	<0.05	<0.05	<0.05
Magnesium	<100	<100	<1	<1	<1	<1	<2
Manganese	96.4	95.9	0.084	0.082	0.106	<0.05	<0.05
Molybdenum	4878	4512	461	453	280	675	1846
Nickel	241530	239083	96.9	95.7	100	80.4	89.5
Palladium	<20	<20	<0.75	<0.75	<0.75	<0.75	<0.75
Phosphorus	116	87.0	2722	2707	2382	568	50.9
Potassium	<10	<10	15.0	14.9	12.1	51.3	10.3
Selenium	<3	<3	<0.1	<0.1	<0.1	<0.1	<0.1
Silicon	<1250	<1250	20.7	22.0	11.4	11.3	7.65
Silver	<1	<1	<0.05	<0.05	<0.05	<0.05	<0.05
Sodium	48.2	16.0	7182	6986	6916	23445	5375
Strontium	<1	<1	<0.05	<0.05	<0.05	<0.05	<0.05
Sulfur	<100	<100	9062	8952	7127	21029	1947
Thallium	<3	<3	<1	<1	<1	<1	<1
Thorium	<100	<100	<0.5	<0.5	<0.5	<0.5	<0.5
Tin	<100	<100	2.32	2.33	1.73	7.66	0.576
Titanium	1688	1669	0.205	0.196	0.220	1.03	0.146
Tungsten	79.7	57.7	2.95	2.96	2.74	8.04	3.33
Uranium	<25	<25	<2	<2	<2	<2	<2
Vanadium	16.6	16.8	<0.1	<0.1	<0.1	<0.1	<2
Yttrium	<1	<1	<0.05	<0.05	<0.05	<0.05	<0.05
Zinc	2.80	2.12	<0.05	<0.05	<0.05	0.062	0.122
Zirconium	<20	<20	0.109	0.095	<0.05	0.071	<0.05

4.4 Anion Analyses of Solid Residue and Treated Liquid Residue

Table 10 presents the anion analyses using ion chromatography of the treated liquid residue samples and a sample of solids labeled as "scale." The analytical data sheets are also given in Appendix G.

Table 10. Anion Analyses of Solid Residue and Treated Liquid Residue.

	Concentration, parts per million (mg/kg for solids, mg/L for liquids)						
	Solids ("scale")		GB Vessels 1 & 2 combined, 01 June		GB Vessel 1 combined from 6 &7 June	H Vessels 1 & 2, 4 June	H Vessel 4 combined from 6 & 7 June
	Original	Duplicate	Analysis	Duplicate			
Anion	163313		162377		162667	162379	162674
Fluoride	<39	<40	29.9	29.7	31.5	48.3	<5.0
Chloride	394970	373974	<5.0	<5.0	<5.0	1846	3034
Nitrite-N	<39	<40	<5.0	<5.0	<5.0	<5.0	<5.0
Nitrate-N	<39	<40	<5.0	<5.0	<5.0	106	181
Sulfate	87.5	96.0	25584	25643	18704	56833	5588

5. Neutralent Simulant

5.1 Feed Composition

Table 11 presents the NMR, anion, and TOC analyses of the neutralent simulant samples submitted by Sandia to SwRI. The accuracy of the NMR analyses, utilizing protocols developed by SwRI, is ± 5 percent. The analytical data sheets for these analyses are presented in Appendix H.

Table 11. Neutralent Simulant Composition.

Analyte	H Neutralent in MEA SwRI ID 163112	GB Neutralent in MEA SwRI ID 163311
Monoethanolamine, MEA	86 percent, by weight	41 percent, by weight
Dichloroethane, DCE	7 percent, by weight	N/A
Dimethyl sulfoxide, DMSO	5 percent, by weight	N/A
Dimethyl methylphosphonate, DMMP	N/A	4 percent, by weight
DMMP "reaction byproduct"	N/A	3 percent, by weight
Hexafluorobenzene	N/A	< 1 percent, by weight
TOC, mg/L	354,000	189,500 Duplicate: 188,500
Fluoride, mg/L	< 10	< 10
Chloride, mg/L	21,341	< 10
Nitrite-N, mg/L	< 10	< 10
Nitrate-N, mg/L	< 10	< 10
Sulfate, mg/L	< 10	< 10
Phosphate, mg/L	< 5	< 5

The DMMP reaction byproduct could not be identified by the NMR analysis. The NMR also failed to detect hexafluorobenzene, which according to the feed specifications, should have been present at a level of 1.6 percent by weight in the GB neutralent simulant. In addition, the anion analyses of the treated GB liquids (Table 10) showed lower than expected fluoride concentrations.

The fluoride ion chromatography analysis presented in Table 11 would only detect "free" fluoride ions in the solution. To measure the total fluoride, the GB neutralent simulant was analyzed utilizing EPA SW-846 Method 5050, "Bomb Preparation Method for Solid Waste." In this method a sample is oxidized by combustion in a bomb (Parr Oxygen Bomb, P/N 1108) containing oxygen under pressure. The liberated compounds are absorbed in a sodium carbonate/sodium bicarbonate solution. The bomb combustate was then analyzed for fluoride using an ion selective electrode. The results of this analysis are presented in Table 12. The analytical data sheet for this analysis is also presented in Appendix HThe total fluoride concentration in the GB neutralent simulant was only about 100 mg/kg (ppm). The liquid density of hexafluorobenzene is approximately 1.6 grams/mL while MEA possesses a density of about 1.0 grams/mL. Thus, thorough mixing of the GB neutralent simulant would be necessary to ensure a homogeneous sample.

Table 12. Total Fluoride in GB Neutralent Simulant by Bomb Combustion

Sample ID	Lab System ID	Fluoride Result (mg/Kg)
Prep Blank	----	<40
Lab Control	----	816
True Value	----	1000
Recovery	----	81.6%
Sandia GB Stimulant	167010	99.9
Duplicate result	167010	106
RPD	167010	5.93%
Spike result	167010	835
Spike added	167010	960
Recovery	167010	76.6%

5.2 Reactor Feed Characterization

Aliquots of the GB and H neutralent simulants provided to SwRI were mixed with the appropriate quantities of sodium hydroxide and hydrogen peroxide to represent the feed solutions for the Batch SCWO process. The "recipes" provided to SwRI for simulating the reactor feeds were as follows:

- H reactor recipe
  - 2.0 grams of H neutralent simulant
  - 0.5 grams of 40 percent sodium hydroxide
  - 28.2 grams of 35 percent hydrogen peroxide

- GB reactor recipe
  - 4.0 grams of H neutralent simulant
  - 1.1 grams of 40 percent sodium hydroxide
  - 29.9 grams of 35 percent hydrogen peroxide

Initial attempts to obtain valid samples of the two feed solutions were complicated by the vigorous reaction that occurred for several hours after the components were mixed. For example, a three-fold batch of each recipe (i.e., approximately 100 grams of materiel) placed into a 1-Liter flask boiled over into the laboratory hood containing the flasks. The reaction was not immediate; the temperature of the solution gradually increased, accompanied by ever increasing release of gas bubbles, until the solution eventually attained the right conditions to boil-over.

Finally, a two-fold batch of each recipe (61.4 grams of H and 70.0 grams of GB) was place into individual 2-Liter flasks. Over a period of several hours, the solutions were allowed to react until the bubbling subsided and it was safe to place the solutions into closed sample containers. No liquid material boiled out of flask, however, the reaction did generate gases that caused a reduction in the original mass of the liquid solutions. The quantities of each liquid recipe recovered from the flasks were 50.7 grams of H (82.6 percent) and 59.6 grams of GB (85.1 percent).

The reactor feeds were analyzed for TOC and NMR. These results were compared to the expected concentrations based upon the raw neutralent simulant analyses (Table 11), and the final weights of the reactor feed samples as discussed in the preceding paragraph. As shown in Table 13, the reactor feed

solutions showed minor decreases in their TOC concentrations and some of their constituent compounds compared to the expected values. Dichloroethane was not detectable in the H reactor solution. The energetic reaction observed subsequent to the mixing of the simulants, caustic, and hydrogen peroxide is believed to be primarily attributable to the degradation of the hydrogen peroxide in the highly alkaline solutions and the release of oxygen. The heat of this reaction, and possibly some oxidation by the hydrogen peroxide, could be reasonably expected to cause the minor reductions in the simulant components.

Table 13. Reactor Solution Composition.

	H Neutralent in MEA Weight percentages		GB Neutralent in MEA Weight percentages	
Analyte	Expected * Reactor Feed	Analysis of Actual Feed	Expected * Reactor Feed	Analysis of Actual Feed
Monoethanolamine, MEA	6.8	5.1	5.5	4.5
Dichloroethane, DCE	0.55	< 0.1	N/A	N/A
Dimethyl sulfoxide, DMSO	0.39	0.4	N/A	N/A
Dimethyl methylphosphonate, DMMP	N/A	N/A	0.54	0.52
DMMP "reaction byproduct"	N/A	N/A	0.40	0.39
TOC, ppm	27,900 ppm	22,800 ppm	25,400 ppm	21,600 ppm

* Based upon original neutralent simulant concentrations reported in Table 11, reactor recipes, and final sample masses of 50.7 and 59.6 grams for H and GB reactor feed samples, respectively.

6. Supplemental Tests for DMMP and DMSO Analyses

Subsequent to the performance test samples, SwRI received seven (7) samples, three labeled for DMMP analysis and four identified for DMSO analysis. All seven (7) samples were found to be below the detection limits for their respective analytes. Table 14 summarizes the data and the analytical data sheets are presented in Appendix H. Since these samples were not fully oxidized materials, a higher sample dilution had to be used for the DMSO analysis to protect the GC/MS instrument.

Table 13. Supplemental Tests for DMMP and DMSO analyses.

Analyte	Vessel #1 DMSO, 163853	Vessel #1 DMMP, 163854	Vessel #2 DMSO, 163855	Vessel #2 DMMP, 163856	Vessel #3 DMSO, 163857	Vessel #4 DMSO 163858	Vessel #4 DMMP 163859
DMMP, µg/L		< 20		< 20			< 20
DMSO mg/L	< 1,000		< 1,000		< 1,000	< 1,000	
TOC, mg/L	12.1	304	11.6	78	94	13.0	518

CLIENT & PROJECT: U.S. Army Program Manager For Chemical Demilitarization Engineering/Design Studies for Treatment of NSCM	PAGE 1 OF 111 TOTAL PAGES: 104
CALCULATION TITLE: **BATCH SCWO VESSEL FEASIBILITY ANALYSIS**	QA CATEGORY (✓) ☐ I ☐ II ☐ III ☑ FEASILILITY STUDY

CALCULATION IDENTIFICATION NUMBER				OPTIONAL
JOB ORDER NO.	DISCIPLINE	CURRENT CALC NO.	OPTIONAL TASK CODE	WORK PACKAGE NO.
10055.37	M	001	NA	NA

APPROVALS – SIGNATURE & DATE			REVISION NO OR NEW CALCULATION NO.	SUPERSEDES CALCULATION NO. OR REVISON NO.	CONFIRMATION REQUIRED (✓)	
PREPARES(S) / DATE(S)	REVIEWER(S) / DATES(S)	INDEPENDENT REVIEWER(S) / DATE(S)			YES	NO
R.A. Weiler	G.Bushnell	G.Bushnell	0			✓

DISTRIBUTION

GROUP	NAME & LOCATION	COPY SENT (✓)	GROUP	NAME & LOCATION	COPY SENT (✓)
Record Mgmt. (or Fire File if none)	R. Mehsling-BA				
Task Manager	J. Cardito				
(Orig.)	A. M. Benigni				

CHANGE HISTORY PAGE

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0	Original			

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1. OBJECTIVE

The objective of this calculation is to evaluate the feasibility of two different Batch SCWO Reactor Vessels. The first unit, referred to as the "Small Vessel", is to be capable of processing CAIS vials. It will be used for testing and could be incorporated into a transportable field unit. A CAIS set would be loaded into the vessel, the vials thermally fractured to expose the agent, and heated to SCWO conditions to destroy the agent. The second unit referred to as the "Large Vessel" is to be of sufficient size to process a typical munition's corresponding neutralent. The Large Vessel is to be a transportable field unit which will also contain the explosive forces associated with accessing and destruction of the munition's burster by explosive means (similar to the EDS-1 unit). The munition would be loaded into the vessel, accessed by explosive shape charges, then heated up to SCWO conditions to destroy the organic material including any remaining energetics.

The specific objectives of this calculation are to determine design, construction and operation feasibility:

- Determine the vessel wall thickness in accordance with ASME Boiler & Pressure Vessel Code, Section VIII, Division1 (Reference 5)
- Determine acceptable heat-up and cool-down rates which could be achieved by conventional external heating/cooling methods
- Determine the fatigue life of the vessels due to thermal and pressure cycling

It is noted that the detailed pressure design and fatigue analysis of the closure head, clamp, and bolting is outside the scope of this study. These components will be designed and fabricated by a suitable vendor who will perform these detailed analyses.

2. METHOD

Vessel wall and closure head thickness is determined from pressure design calculations performed in accordance with the ASME Boiler and Pressure Vessel Code, Section VIII, Division1 (Reference 5).

The vessel response to thermal heat-up and cool-down transients is calculated using the ANSYS/Mechanical (Reference 6) general purpose finite element code. An axisymmetric model of the vessel shell, closure head, clamp and lower head is constructed using ANSYS PLANE55 elements. The PLANE55 is a 2-D thermal solid element which has thermal conduction capability for both steady-state and transient analyses.

The heat-up transient is simulated by setting the initial model temperature to room temperature (70°F), and applying a heat flux to the outer surfaces of the model. A transient solution is then run and the resulting thermal gradients and end of transient temperatures reviewed. The heat flux and transient length is then adjusted and the model is rerun. Using an iterative procedure a reasonable heat-up solution is determined. This solution is later confirmed to be acceptable by the fatigue analysis.

The cool-down transient is simulated by setting the model temperature at 1200°F and applying a forced convection (air) film coefficient and a bulk temperature of 70°F to the outer model surface. A transient solution is performed until the model approaches room temperature.

To determine vessel stresses due to both internal pressure and thermal gradient loads the ANSYS model is converted to PLANE42 axisymmetric 2-D structural solid elements. Internal pressure is applied to the inner surfaces of the model and the resulting stress distribution is calculated. For thermal stresses calculations the nodal temperature distribution from selected heat-up and cool-down time steps is applied and a stress solution obtained.

To determine vessel fatigue life a design fatigue curve is developed in accordance with ASME Boiler and Vessel Code, Article III-2000 using vendor supplied fatigue test data. This was necessary since no design fatigue is available for the vessel alloy at the operating temperatures required. Using the ANSYS finite element results for the heat-up, cool-down, and pressure cases the resulting stress range is calculated and the allowable number of operational cycles is determined from the design fatigue curve.

The ANSYS analyses are performed on Stone & Webster workstation #00335, running the Windows NT 4.00.1381 operating system.

3. ASSUMPTIONS

- Shells are assumed seamlessforgings (available as SB-564)
- SCWO conditions are assumed to envelope explosive accessing and buster destruction conditions in the large vessel (based on dimensional comparisons with and explosive test responses of EDS-1, Reference 7)
- EDS-1 internals including support tray and shrapnel containment are assumed to be directly applicable for use in the large vessel
- Assumed geometry of clamped flange closure head based on catalog data (Attachment A)
- Thermal resistance of Zirconium liner is neglected

4. INPUTS

4.1 Material Properties for Alloy UNS N06617

Table 4.1-1
Nominal Chemical Composition, %,
INCONEL Alloy 617
(Reference 1)

Nickel	52.0
Chromium	22.0
Cobalt	12.5
Molybdenum	9.0
Aluminum	1.2
Carbon	0.07
Iron	1.5
Manganese	0.5
Silicon	0.5
Sulfur	0.008
Titanium	0.3
Copper	0.2

Table 4.1-2
Physical Constants
(Reference 1)

Density, $lb/in.^3$ 0.302

Melting Range, °F 2430-2510
°C 1332-1377

Specific Heat at 78°F (26°C)
Btu/lb.-°F 0.100

Table 4.1-3
Thermal Properties
(Reference 1)

Temperature	**Thermal Conductivity**	**Coefficient of Expansion**	**Specific Heat**
°F	**Btu-in/ft^2-h-°F**	**10^{-6}in./in./°F**	**Btu/lb.°F**
78	94	-	0.100
200	101	6.4	0.104
400	113	7.0	0.111
600	125	734	0.117
800	137	7.6	0.124
1000	149	7.7	0.131
1200	161	8.0	0.137
1400	173	8.4	0.144
1600	185	8.7	0.150
1800	197	9.0	0.157
2000	209	9.2	0.163

Table 4.1-4
Physical Properties
(Reference 1)

Temperature	**Tensile Modulus**	**Shear Modulus**	**Poisson's Ratio**
°F	**10^6 psi**	**10^6 psi**	
74	30.6	11.8	0.30
200	30.0	11.6	0.30
400	29.0	11.2	0.30
600	28.0	10.8	0.30
800	26.9	10.4	0.30
1000	25.8	9.9	0.30
1200	24.6	9.5	0.30
1400	23.3	9.0	0.30
1600	21.9	8.4	0.30
1800	20.5	7.8	0.31
2000	18.8	7.1	0.32

4.1 Dry Air Properties

At 200 °F (Reference 2):

$\rho = 0.0601\ lb_m/ft^3$

$C\rho = 0.242\ Btu/lb_m\ F$

$K = 0.018\ Btu/hr\ ft\ F$

$\mu = 0.052\ lb_m/hr\ ft$

$\nu = 0.864\ ft^2/hr$

$Pr = 0.694$

4.2 Fatigue Data for UNS NO6617

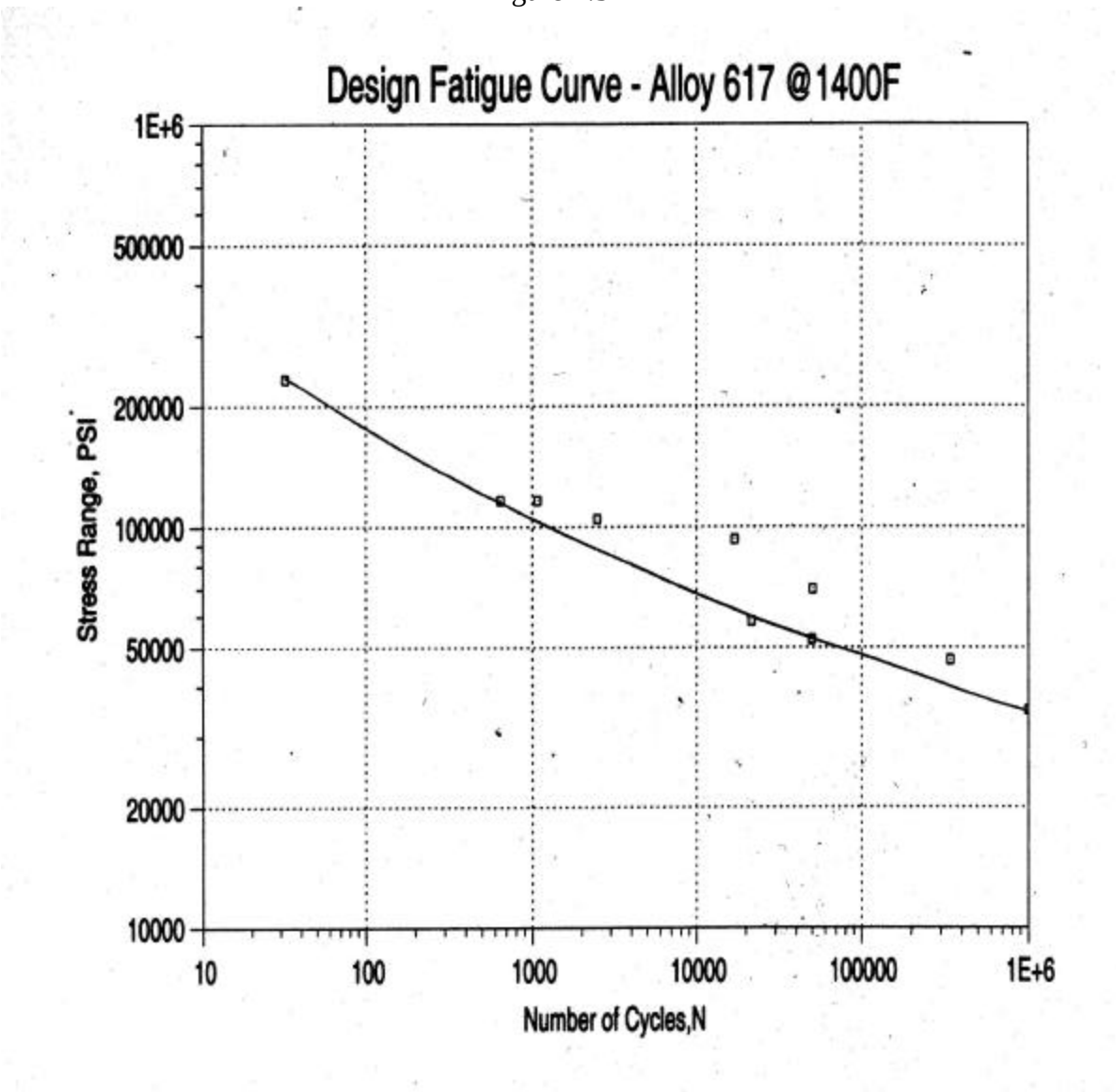
Table 4.3-1 Alloy 617 Low Cycle Fatigue Data 1400°F
(Reference 3)

Total Strain Range Pct	First Cycle $\Delta\sigma$ Ksi	Mid-Life $\Delta\sigma$ Ksi	N_i Cycles	N_f Cycles	H
1.0	85.7	122.2	648	2,671	29.9
0.50	71.4	99.2	21,618	26,331	28.0
0.45	72.0	98.1	49,844	50,244	26.6
0.40	79.0	89.1	341,920	349,262	11.3
0.30	64.8	70.4	Removal at 1,009,900		8.0

Table 4.3-1 - Total strain data for INCONEL alloy 617 at 1400F presenting total stress $\Delta\sigma$ at first and mid-life cycles, the number of cycles to crack initiation (N_i) and to failure (N_f) and the degree of hardening (H).

A design fatigue curve, Figure 4.3-1, is generated from the fatigue data of Table 4.3-1 in accordance with ASME Boiler & Pressure Codes Article III-2000, Paragraph III-2200 (Reference 5). The design stress intensity values are obtained from the best fir curve by applying a factor of 2 on stress or a factor of 20 on cycles, whichever is the more conservative at each point.

Figure 4.3-1


Design Fatigue Curve - Alloy 617 @1400F
Stress Range, PSI
1E+6
500000
200000
100000
50000
20000
10000
10
100
1000
10000
100000
1E+6
Number of Cycles,N

4.3 Batch SCWO Design Basis for Vessels

(Reference 4)

Small Vessel

Reactor Volume	**Pressure**
3 gallon	6221 psi
4 gallon	4900 psi
5 gallon	4100 psi[1]

Large Vessel

Reactor Volume	**Pressure**
403 liters	4000 psi
306 liters	5000 psi
240 liters	6000 psi

[1] For the analysis in this calculation, a pressure of 4000 psi was used with a 5 gallon volume for the small vessel. This will have an insignificant effect on the results of this calculation.

5. SUMMARY OF RESULTS/CONCLUSIONS

The following table summarizes the results of the Batch SCWO vessel feasibility analysis. The heatup and cooldown rates will support processing of one operational cycle in a 24 hour period using external ceramic fiber heaters for heatup and forced convection for cool down. Fatigue life exceeds 2 years based on one cycle per day, 5 days a week operational period. It is concluded that each batch SCWO vessel design is feasible for the intended use and does not require significant technology or fabrication process development for implementation.

Batch SCWO Vessel Feasibility Study Results

Parameters		Large Vessel	Small Vessel
Design Conditions:	Pressure	4000 psi	4000 psi
	Temperature	1250 F	1250 F
Vessel Description:	Capacity	106 Gallon (400L)	5 Gallon (19L)
Cylindrical Shape with a Flat Head and Closure	Material	UNS N06617 Ni-Cr-Co-Mo Alloy	UNS N06617 Ni-Cr-Co-Mo Alloy
	Corrosion Barrier	Zirconium (Alloy 702)	Zirconium (Alloy 702)
	Shell	20.0" ID	7.75" ID
	Shell Length	78"	24"
	Shell Wall Thickness	3.875"	1.5"
	Lower Head	6.375" thick	2.5" thick
	Closure[2]	REFLANGE G-CON 8" thick	REFLANGE G-CON 4.75" thick
Weight:	Closure	1750 lbs.	150 lbs.
	Clamp	1500 lbs.	140 lbs.
	Shell	7000 lbs.	320 lbs.
	Bottom Head	1250 lbs.	90 lbs.
	Total	11,500 lbs.	700 lbs.
SCWO Heatup:	Power Input	7 to 15 watts/sq. in, 70 kW Total	7 to 20 watts/sq. in, 10 kW Total
Ceramic Fiber Heating Elements	Heatup Time	5 Hours	2 Hours
SCWO Cooldown:	Air Velocity	50 to 60 ft/sec	50 to 60 ft/sec
Forced Convection By Air	Cooldown Time	13 Hours	5 Hours
Fatigue Life:	Stress Range	110 ksi	95 ksi
	Allowable Cycles	700	1,600

[2] Closure detailed design shall be determined by vendor.

6. REFERENCES

1. INCO Alloy International. *Solutions to Materials Problems.* 1997.
2. Rohsenow, Warren M. & Harry Choi. *Heat, Mass, and Momentum Transfer.* New Jersey: Prentice-Hall, 1961, p. 522.
3. Alloy 617 Low Cycle Fatigue Data 1400°F from INCO Alloys International.
4. Batch SCWO Design Basis (unissued - included as Attachment C).
5. ASME Boiler & Pressure Vessel Code, Section VIII, Division I, 1998 Edition with Addena through 2000.
6. ANSYS/Mechanical (ST-384.1), ANSYS, Inc., Release 5.5.1.
7. Explosive Destruction System Phase 1 Interim Test Report, December 20, 2000.
8. Material Selection For Batch SCWO Processing (included as Attachment D).

7. CALCULATION BODY

7.1 Conceptual Design of Vessels

The Batch SCWO vessels are cylindrical in shape with flat heads to facilitate the incorporation of penetrations. A clamp type closure (Example REFLANGE G-CON) is selected for to facilitate removal of the head during operation. G-CON flanges are shown in Attachment A.

The Small Vessel is required to be in the 3 to 5 gallon range (Section 4.4). In order to minimize the design pressure requirements and resultant wall thickness, the 5 gallon vessel capacity was selected. An inner diameter of 7.75" was chosen to match the inner diameter of a 10" F10-1.5 G76 REFLANGE G-CON buttweld hub. A matching G-CON blind hub and clamp are chosen for the closure (assuming SB-564 material).

The Large Vessel is required to be a minimum of 63 gallons (Section 4.4). An internal diameter of 20" is chosen to match the EDS Phase 1 vessel to allow incorporation of the same fragment suppression system. A 106 gallon capacity is selected to minimize the design pressure and resultant wall thickness. A custom designed hub/blind hub/clamp will be required. For dimensional purposes a 24" REFLANCE G-CON closure is used (assuming SB-564 material).

For operational considerations, both vessels are oriented horizontally. Handling and positioning provisions for the closure head and closure supports are not integral to the pressure boundary. For corrosion protection considerations a Zr-702 liner is required to insulate the pressure boundary material from the reaction products. Intermediate and final by-products of agent neutralization and SCWO destruction yield acids that are highly aggressive to nickel alloys. The liner is conceptualized as a thin (≈ 0.05"), close-fitting but non-integral member that similar to cladding, extends over the closure surfaces. Final forming is obtainable by several methods including hydrostatic and Magnaform™.

The method of heating of the vessels was chosen to be electric ceramic fiber heating elements. Conceptually, the heaters would be supported in a space frame structure which standing off the vessel by 1" to 2". This type of heater/mounting system is manufactured by Watlow and is shown in Attachment B. The annulus between the heaters and the vessel serve as a flow path for the forced convection air cooling system. Conceptually an exhaust fan would be connected by ductwork to the annulus to draw cooling air across the vessel surfaces.

7.2 ASME Code Pressure Design for Batch SCWO Vessels

(Reference 5)

Design Conditions for Vessels: Pressure = 4000 psi
Temperature = 1250 °F

Material: SB – 564 (UNS NO6617)
S_y = 35 ksi
S_u = 95 ksi
S = 13.0 ksi @ 1250°F

Geometry: Vertical Vessel
Flat Head at bottom
Flat Head at top with clamped flange

Minimum Required Wall Thickness (UG-27):

$P \leq 0.385SE$ ($\leq$ 4000 psi)

$t = (P*R)/[(S*E) – (0.6*P)]$

where, t = minimum required thickness of shell, in
P = internal design pressure, psig
R = inside radius of the shell course under consideration
S = maximum allowable stress value, psi
E = 1.0, joint efficiency for appropriate joint in shells (UW-12) - longitudinal joints

Small Vessel: t = 1.46” use 1.5”
Large Vessel: t = 3.77” use 3.875”

Minimum Required Head Thickness (UG-34):

$t = d*[(C*P)/(S*E)]$

where, t = minimum required thickness of flat head or cover, in
d = diameter
C = 0.2, a factor depending upon the method of attachment of head, shell dimensions, etc.
P = internal pressure design, psig
S = maximum allowable stress value in tension, psi
E = 0.9, joint efficiency - circumferential joints

$r_{MIN} = (1/4)*t_{shell}$, transition radius between shell and head

Small Vessel: t_{MIN} = 2.03”

Large Vessel: r_{MIN}= 0.75
t_{MIN} = 5.23”
r_{MIN} = 1.0”

7.3 ANSYS Model Geometry and Plots

The ANSYS model geometry is shown in Figures 7.3-1 and 7.3-2 and plots of the models are shown in Figures 7.3-3 and 7.3-4. The ANSYS models are axisymmetric finite element representations of the vessel geometry. The vessel modeling of the shell and lower head reflect the geometry derived in Sections7.1 and 7.2. The detailed geometry of the closure head, flange, clamp, and bolting is not known at this time and these components are approximated in the ANSYS models. The intent is to include the effects of these components both thermally and structurally to the extent that they affect the results on the vessel shell and lower head. The detailed pressure design and fatigue analysis of the closure head, clamp, and bolting is outside the scope of this calculation. These components will be designed and supplied by a suitable vendor who will perform these analyses.

Figure 7.3-1: Small Vessel Geometry

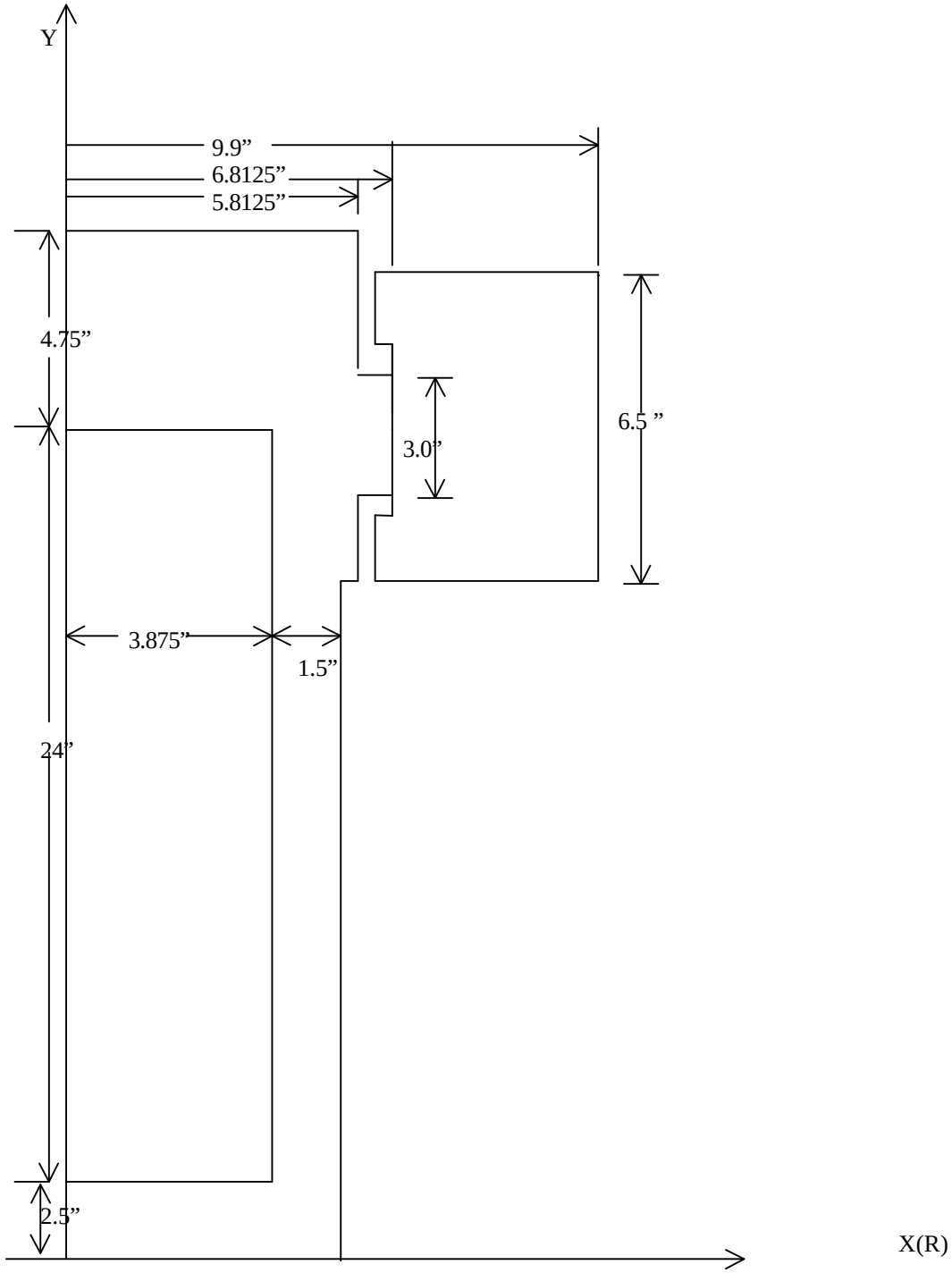


Figure 7.3-2: Large Vessel Geometry

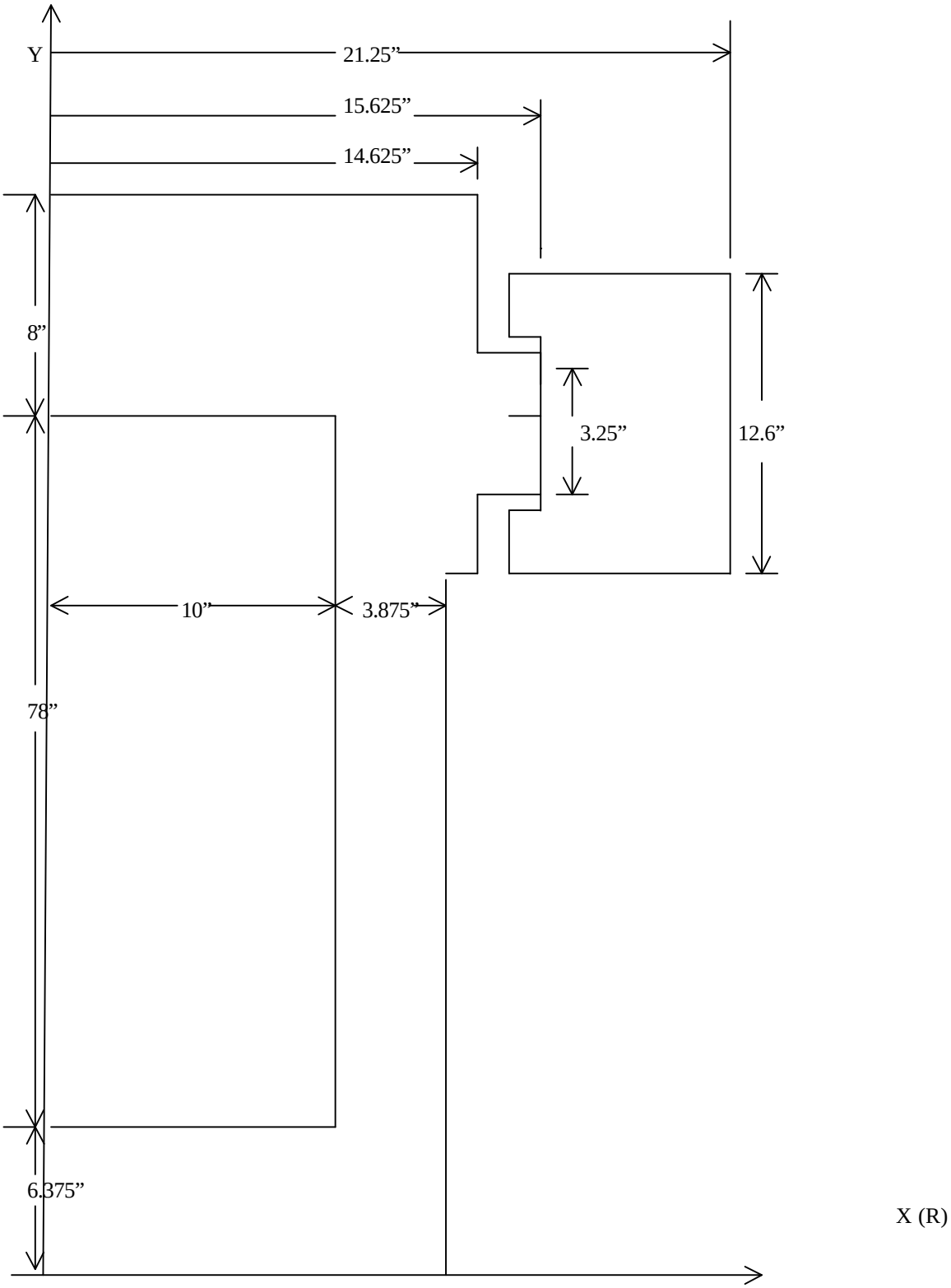
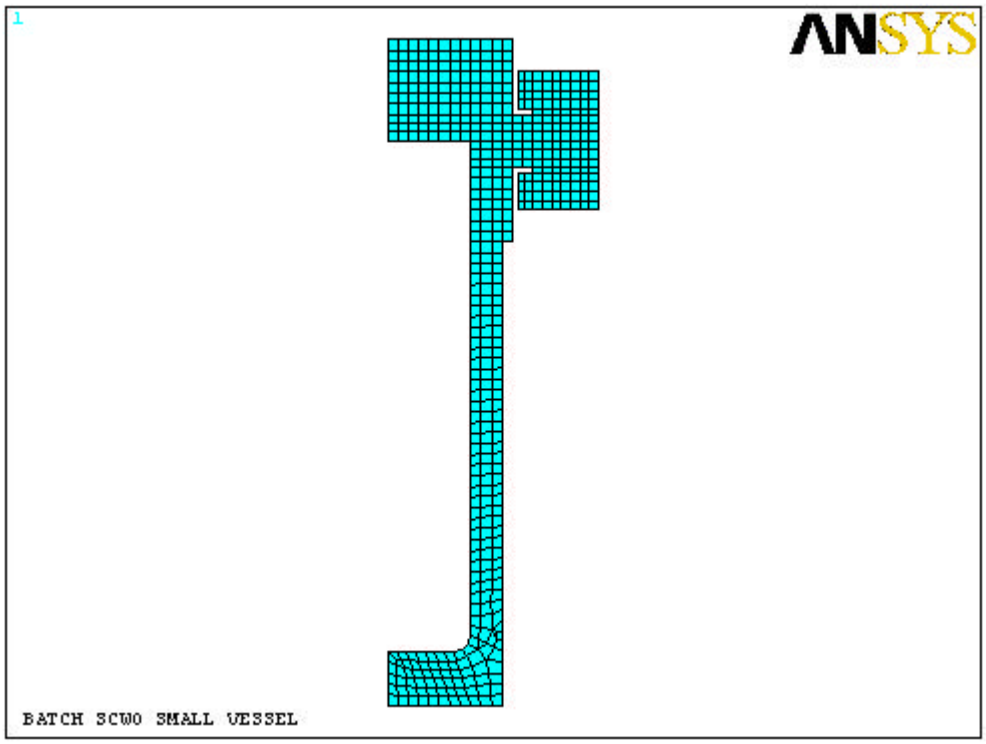


Figure 7.3-3: Small Vessel ANSYS Model



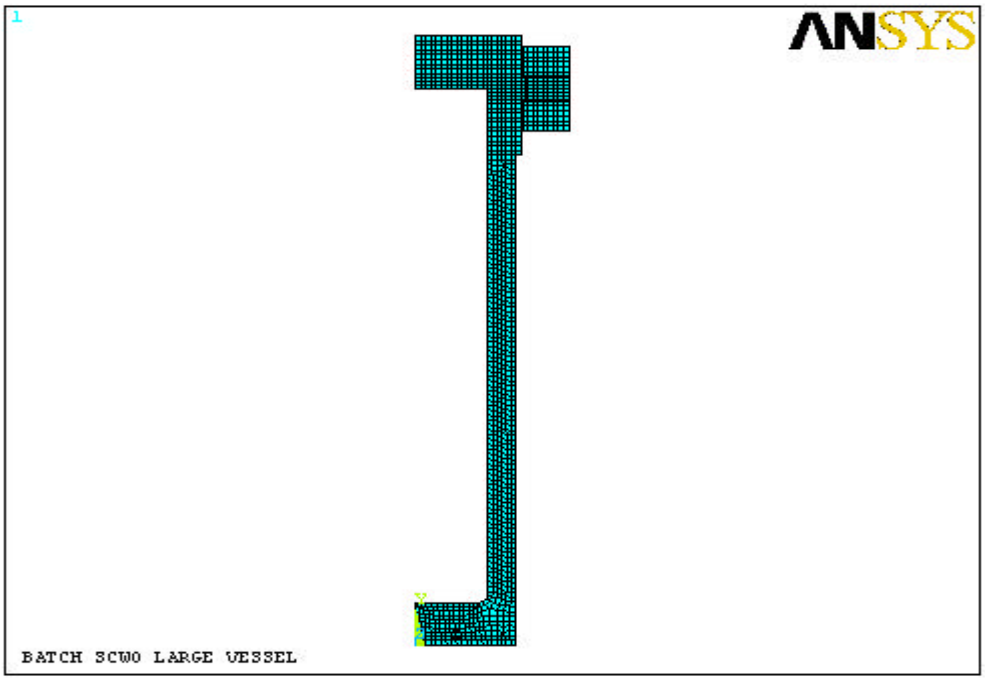


Figure 7.3-4: Large Vessel ANSYS Model

7.4 Weights of Vessel Components

Small Vessel

Closure = $\pi * 5.8175^2 * 4.75 * 0.302 = 152$ lbs.	Use 150 lbs.
Clamp = G-CON Cx8 = 135 lbs.	Use 140 lbs.
Shell = $\pi * (5.375^2 - 3.875^2) * 24 * 0.302 = 316$ lbs.	Use 320 lbs.
Bottom Head = $\pi * 5.8175^2 * 2.5 * 0.302 = 68$ lbs.	Use 90 lbs.
Total Weight = 671 lbs.	**Use 700 lbs.**

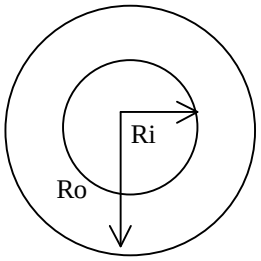
Large Vessel

Closure = $\pi * 14.625^2 * 8.0 * 0.302 = 1623$ lbs.	Use 1750 lbs.
Clamp = G-CON C3Y = 1500 lbs.	Use 1500 lbs.
Shell = $\pi * (13.875^2 - 10.0^2) * 78 * 0.302 = 6846$ lbs.	Use 7000 lbs.
Bottom Head = $\pi * 13.875^2 * 6.375 * 0.302 = 1164$ lbs.	Use 1250 lbs.
Total Weight = 11,133 lbs.	**Use 11,500 lbs.**

7.5 Calculation of Heat Transfer Coefficient for Forced Convection (Cooldown)

Small Vessel

For an annulus:



Ri = 5.375”
Ro = 6.375”

For air @ 200°F (Reference 3):

$\rho = 0.0601$ lb_m/ft^3
$C\rho = 0.242$ Btu/lb_m F
K = 0.018 Btu/hr ft F
$\mu = 0.052$ lbm/hr ft
$\nu = 0.864$ ft^2/hr
Pr = 0.694

Let Velocity = 50 ft/sec

Equivalent Diameter = 4 * (flow area/wetted perimeter)

$De = 2*[(Ro^2-Ri^2)/(Ro+Ri)]$
De = 2*(11.75 in/11.75 in)
De = 2.0 in

Reynolds Number = (De*V*ρ)/μ

Re = [(2in*50ft/sec*0.0601lb_m/ ft^3)/(0.052 lb_m/hrft)]*(1ft/12in)*(3600sec/hr)

Re = 34,673

Heat Transfer Coefficient = $0.037*Re^{0.8}*Pr^{1/3}$

$N_u = 0.037*(34{,}673^{0.8})*(0.694^{1/3})$

$N_u = 140$

Equivalent Diameter = 4 * (flow area/heated perimeter)

$De = 2*[(Ro^2-Ri^2)/(Ri)]$

De = 2*(11.75in/5.375in)

De = 4.372 in

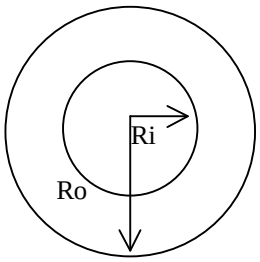
Heat Transfer Coefficient = (K* N_u)/(De)

H = [(0.018Btu/hr ft F * 140)/(4.372in)]*(12in)

H = 6.9 Btu/hr ft^2 F

Large Vessel

For an annulus:



Ri = 5.375”

Ro = 5.875”

For air @ 200°F (Reference 3):

ρ = 0.0601 lb_m/ft^3

Cρ = 0.242 Btu/lb_m F

K = 0.018 Btu/hr ft F

μ = 0.052 lbm/hr ft

ν = 0.864 ft^2/hr

Pr = 0.694

Let Velocity = 50 ft/sec

Equivalent Diameter = 4 * (flow area/wetted perimeter)

$De = 2*[(Ro^2-Ri^2)/(Ro+Ri)]$

De = 2*(5.625 in/11.25 in)

De = 1.0 in

Reynolds Number = (De*V*ρ)/μ

Re = [(1in*50ft/sec*0.0601lb_m/ ft^3)/(0.052 lb_m/hrft)]*(1ft/12in)*(3600sec/hr)

Re = 17,336

Heat Transfer Coefficient = $0.037*Re^{0.8}*Pr^{1/3}$

$N_u = 0.037*(17{,}336^{0.8})*(0.694^{1/3})$

$N_u = 81$

Equivalent Diameter = 4 * (flow area/heated perimeter)

$De = 2*[(Ro^2-Ri^2)/(Ri)]$

De = 2*(5.625in/5.375in)

De = 2.10 in

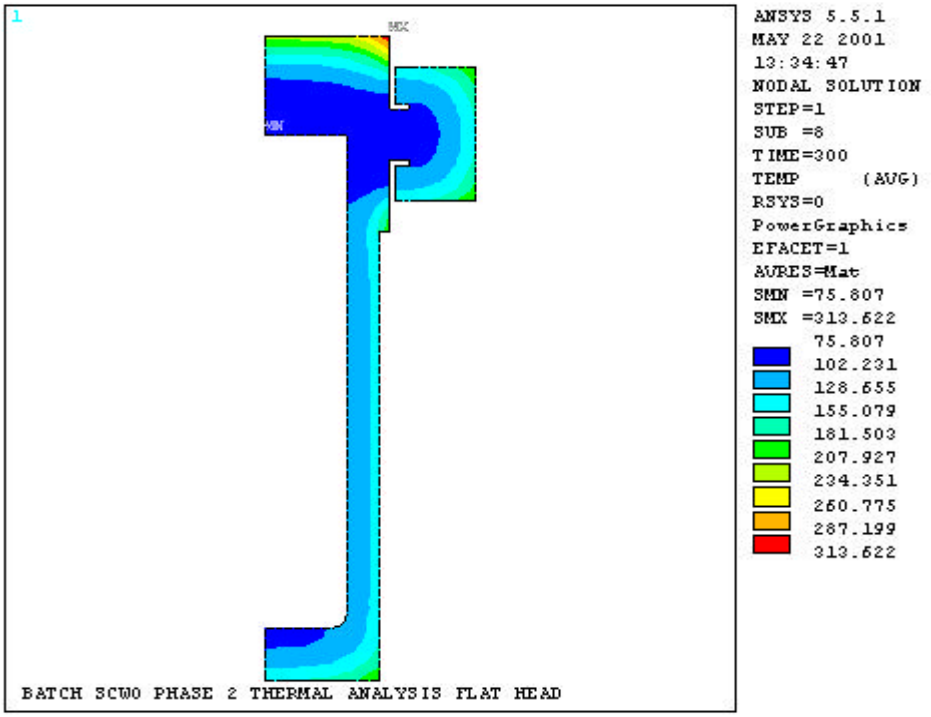
Heat Transfer Coefficient = $(K* N_u)/(De)$

H = [(0.018Btu/hr ft F * 81)/(2.10in)]*(12in)

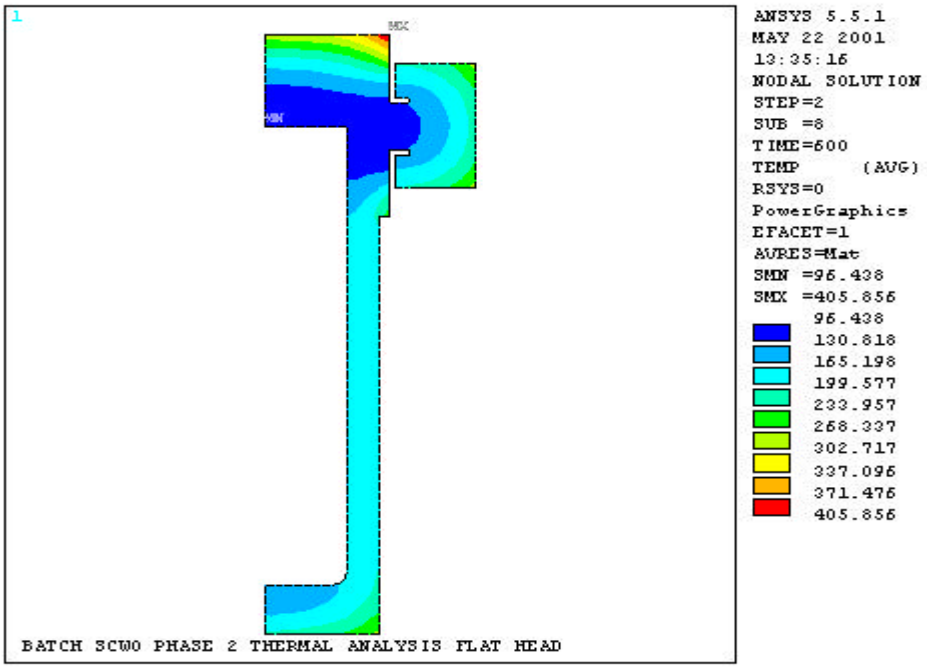
H = 8.3 Btu/hr ft^2 F

7.6 Small Vessel Thermal Contour Plots – Heatup Transient

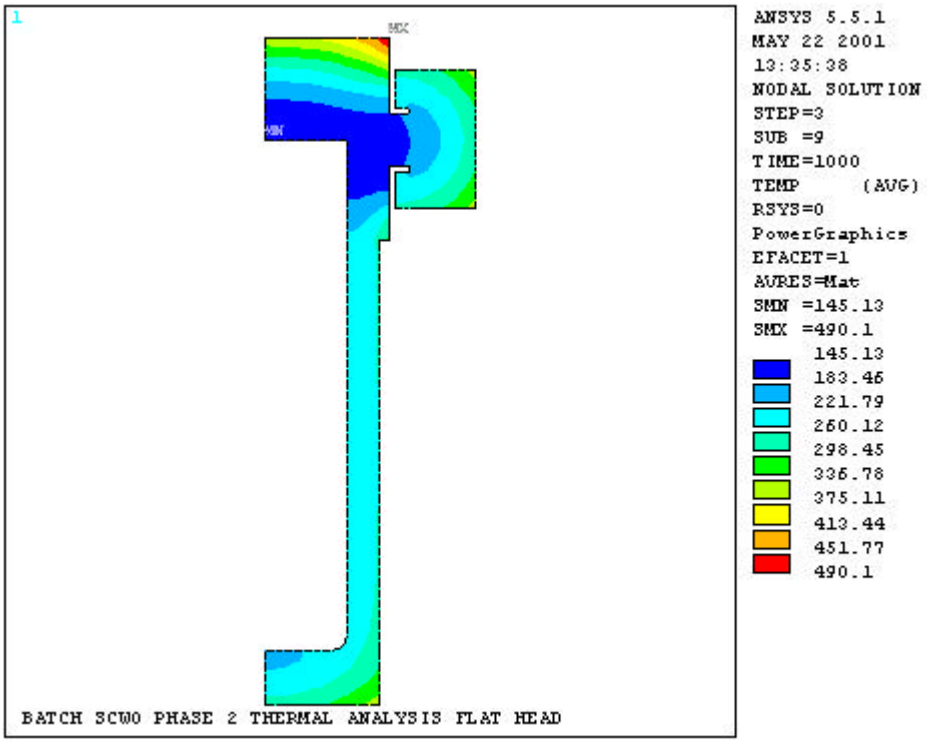
The temperature contour plots contained in this section are for selected time steps in the ANSYS solution for the small vessel heat-up transient. Heat flux input loading varies between 7 watts/sq. in along the vessel shell and 15 watts/sq. in at the heads. The model is initially at 70°F and the heat flux is applied as a constant value until 6500 sec where it is removed. The model is allowed to equilibrate until 7200 sec. As can be seen in the plots the model is between 1045°F and 1180°F at 7200 sec.



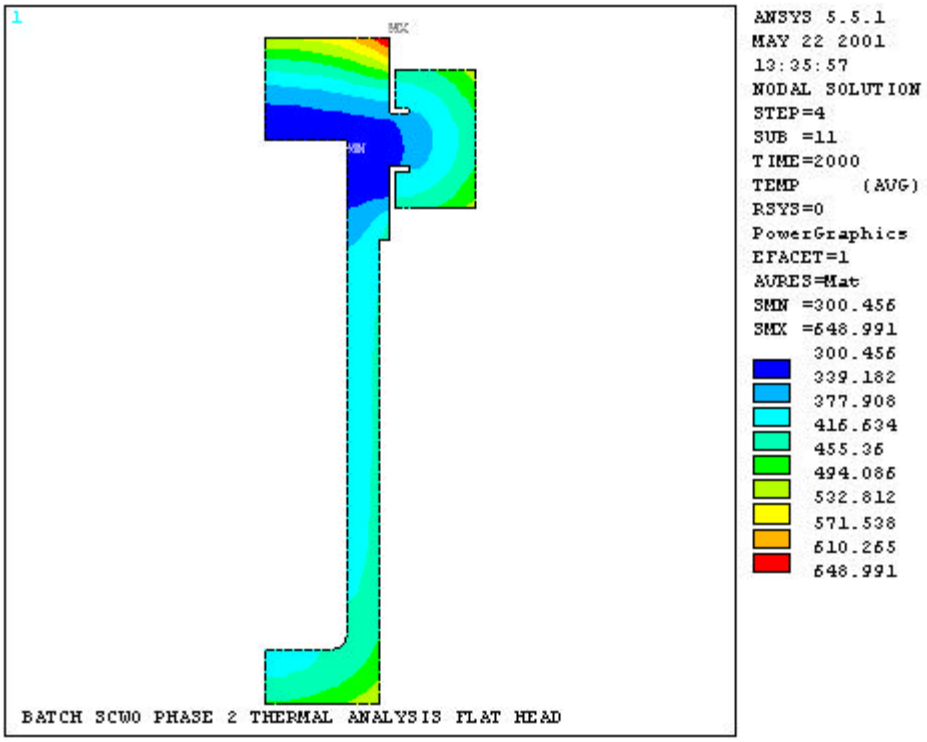
Batch SCWO Small Vessel Heatup 300 sec



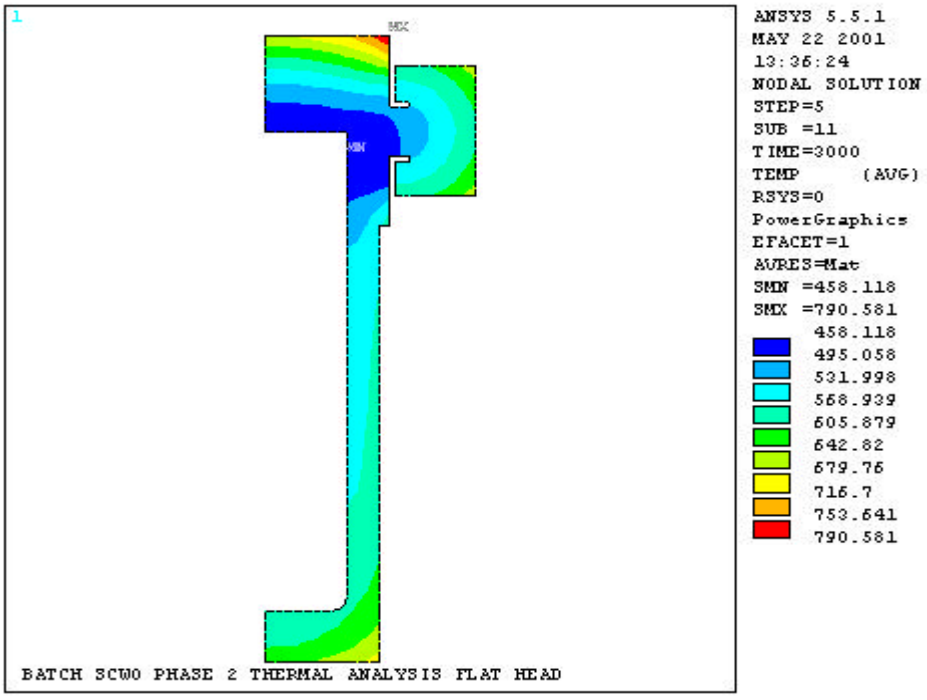
Batch SCWO Small Vessel Heatup 600 sec



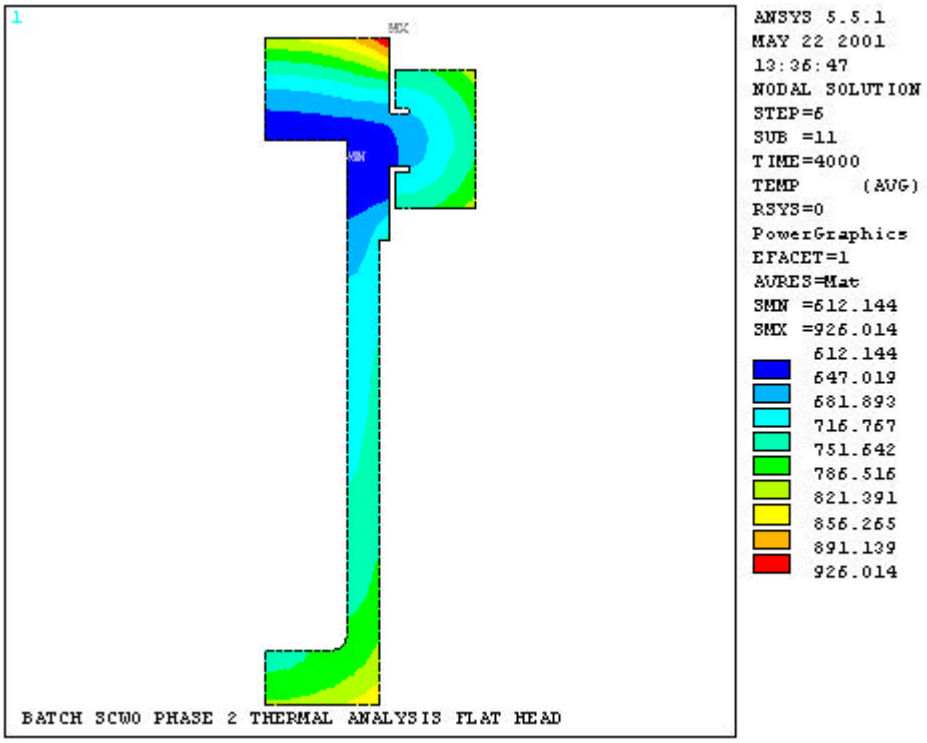
Batch SCWO Small Vessel Heatup 1000 sec



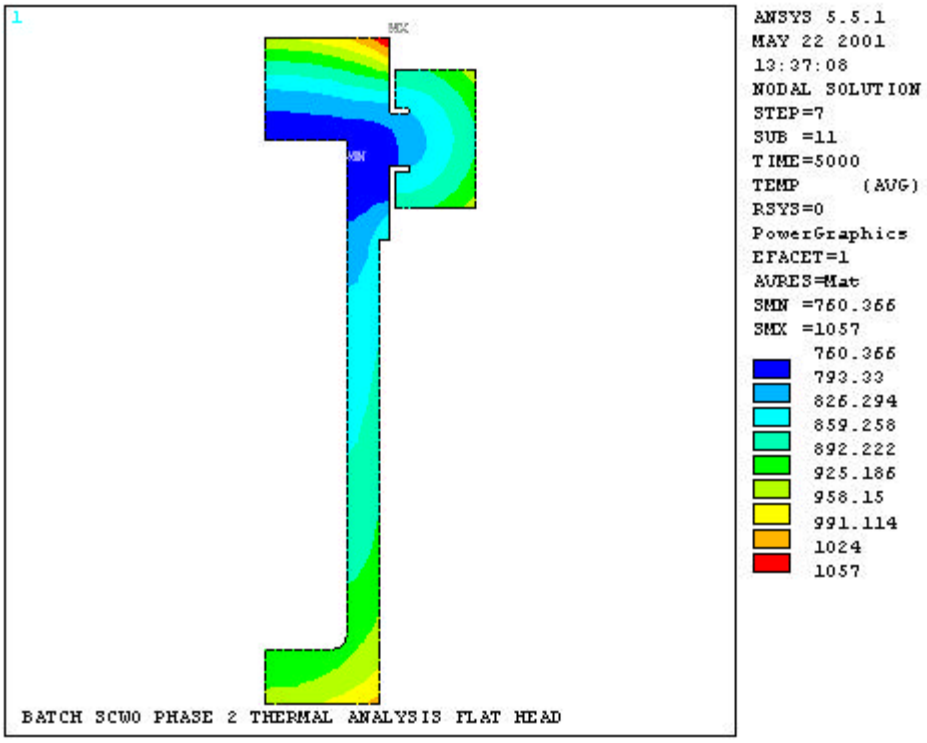
Batch SCWO Small Vessel Heatup 2000 sec



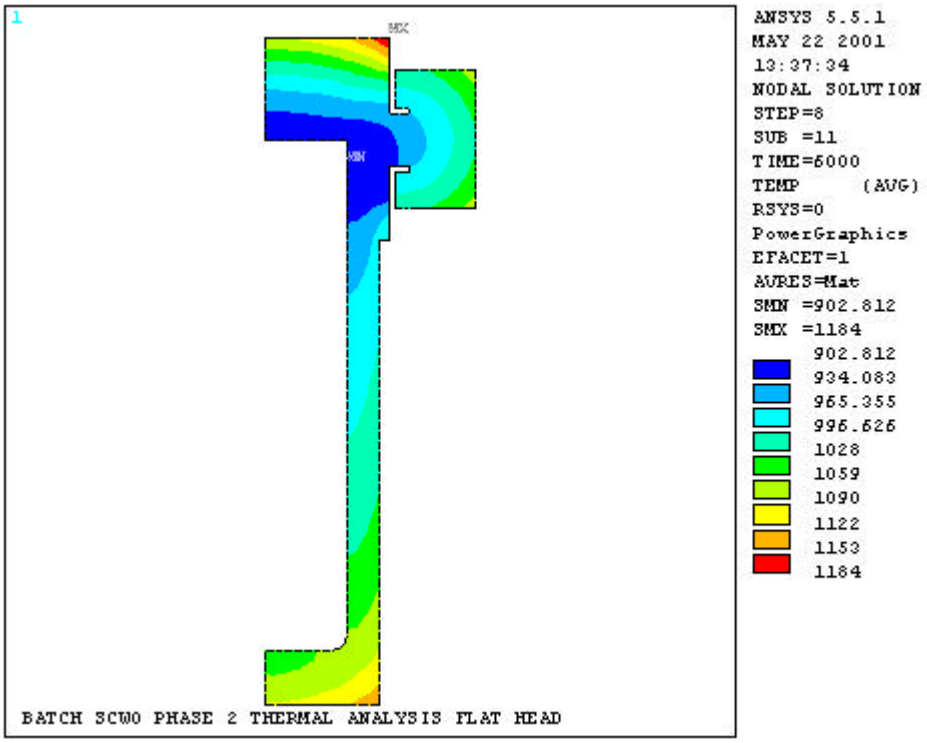
Batch SCWO Small Vessel Heatup 3000 sec



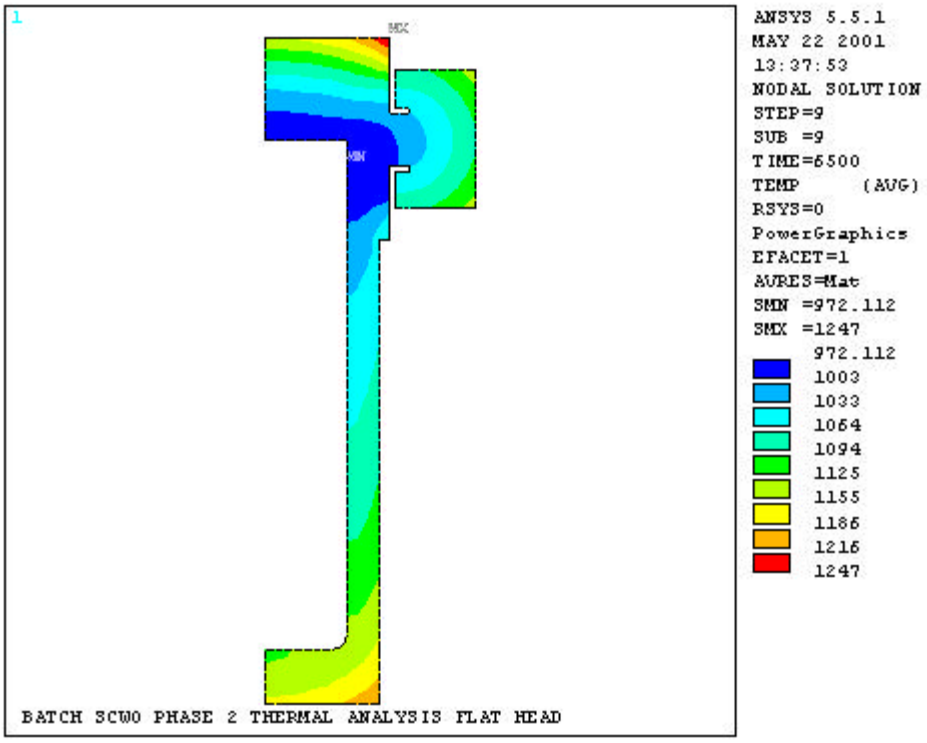
Batch SCWO Small Vessel 4000 sec



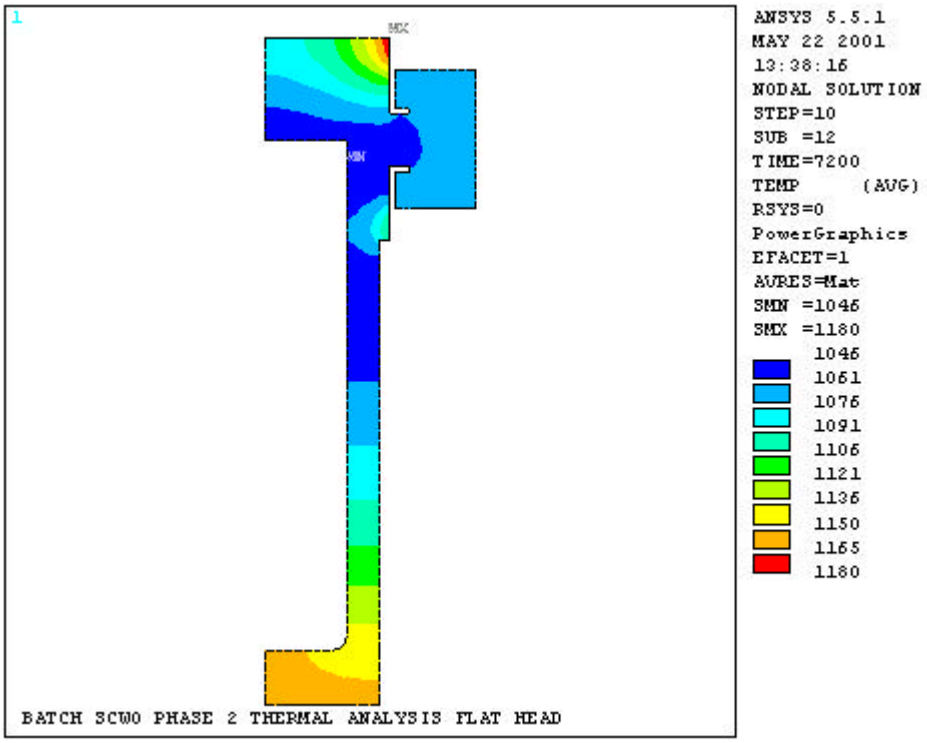
Batch SCWO Small Vessel 5000 sec



Batch SCWO Small Vessel 6000 sec



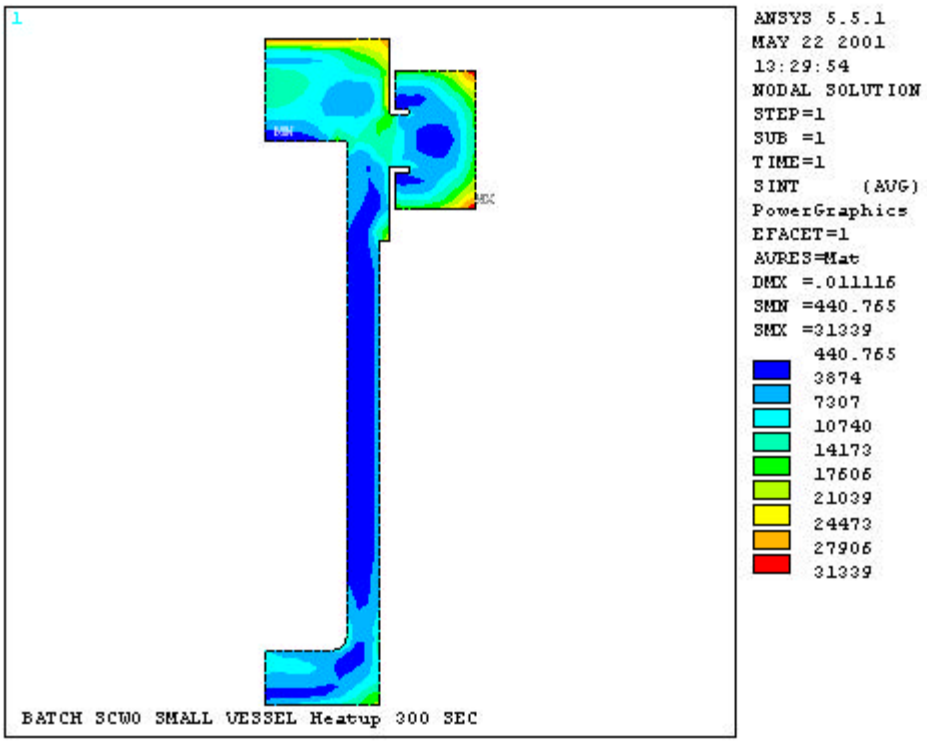
Batch SCWO Small Vessel 6500 sec

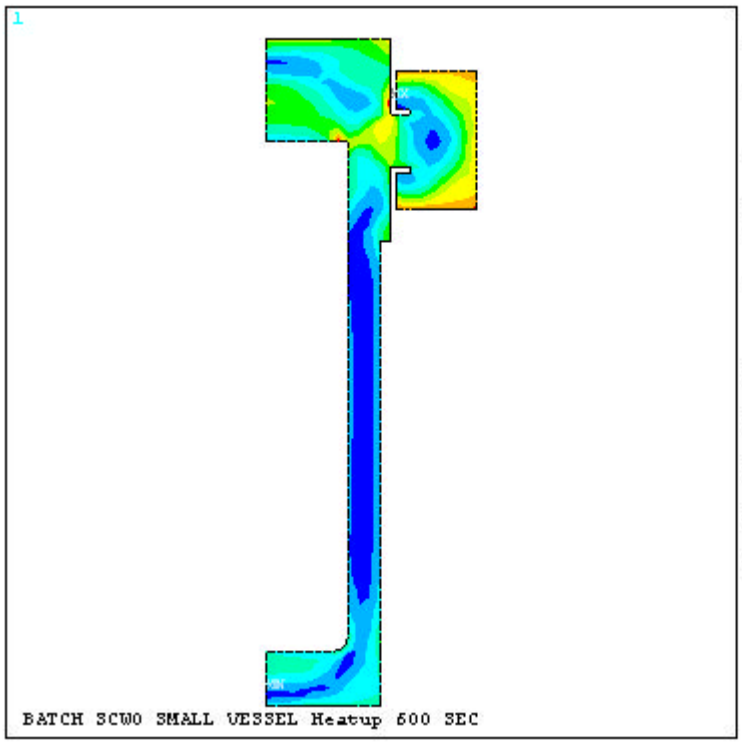


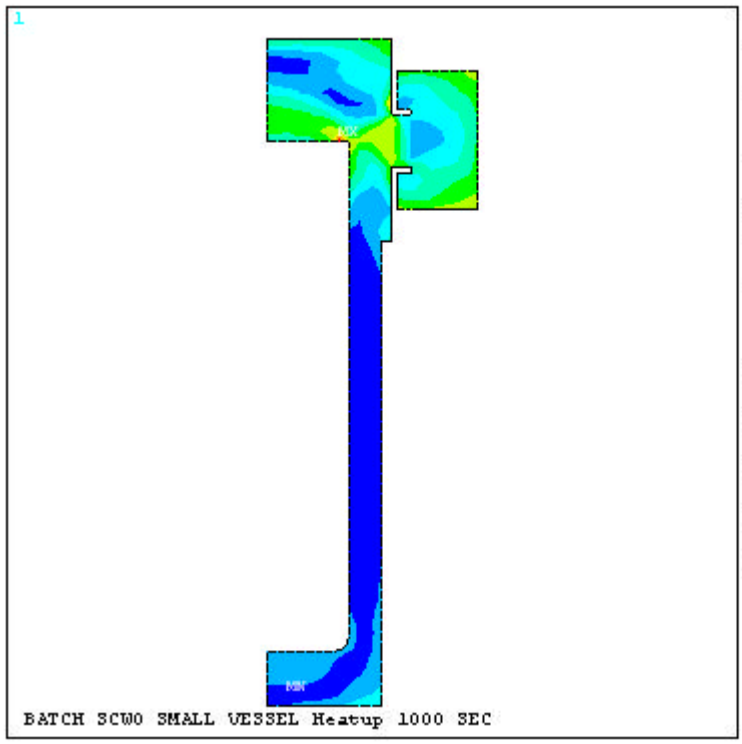
Batch SCWO Small Vessel 7200 sec

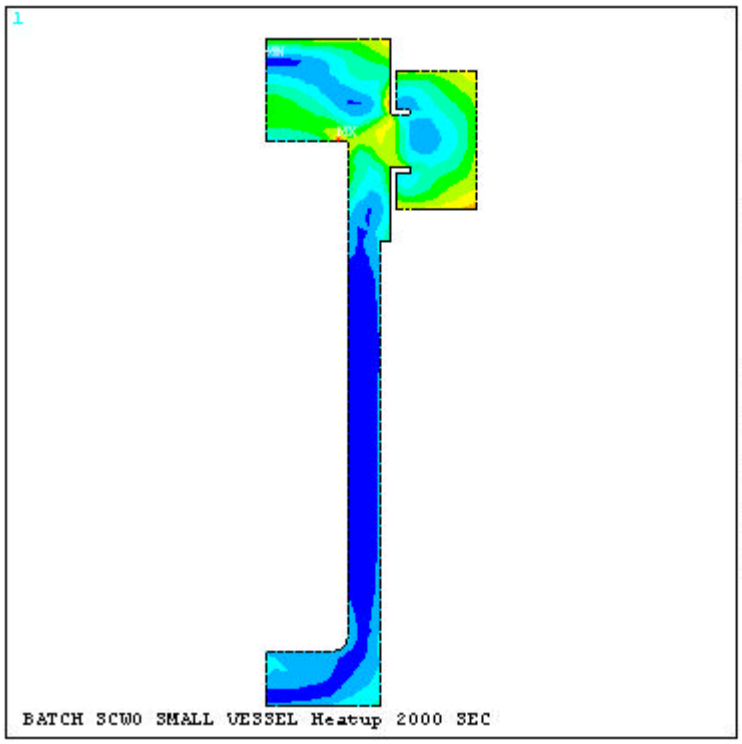
7.7 Small Vessel Stress Contour Plots – Heatup Transient

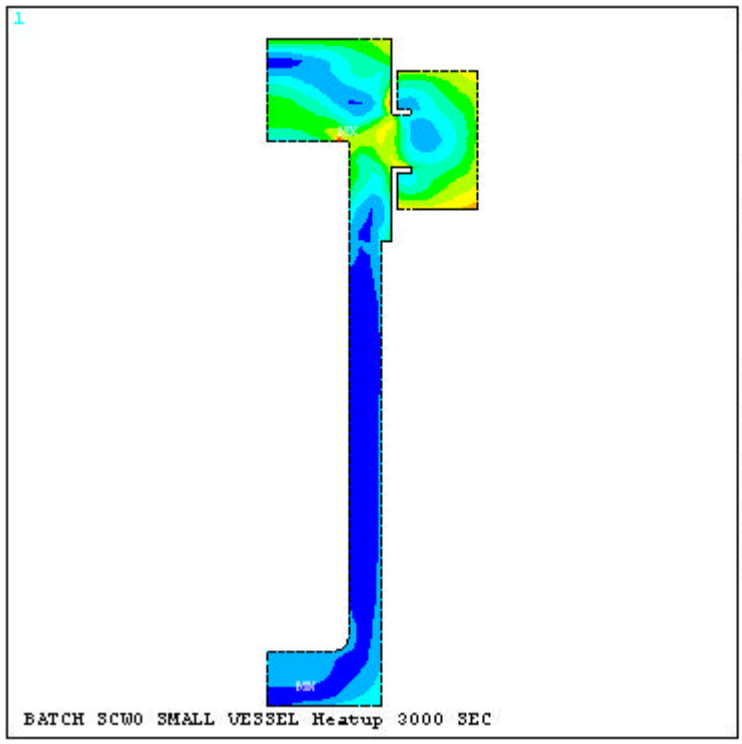
The stress intensity contour plots contained in this section are calculated for the temperature distribution corresponding to the selected time steps in the ANSYS solution for the small vessel heat-up transient. The maximum stress intensity is located on the inside surface of the head, occurs at 1000 sec. and is equal to 45355 psi.

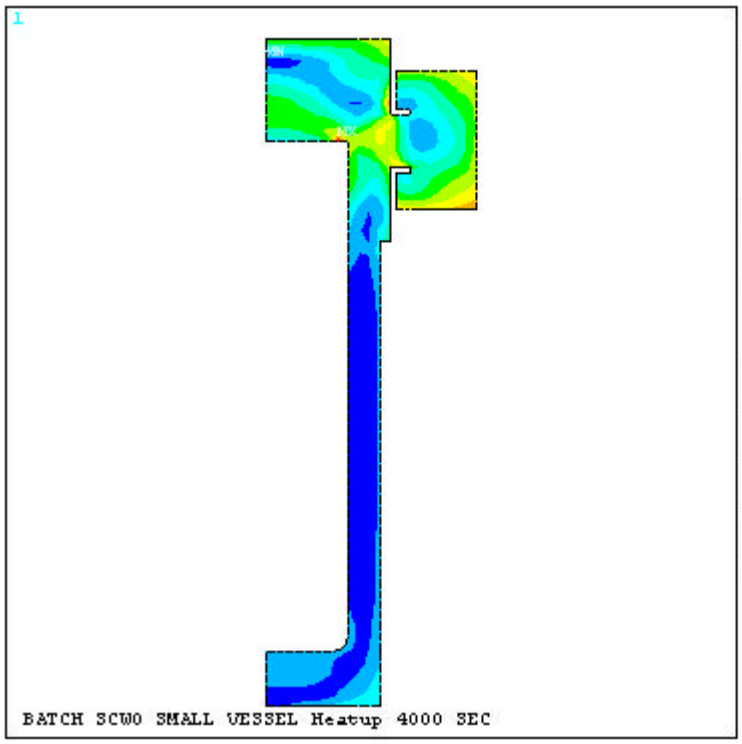


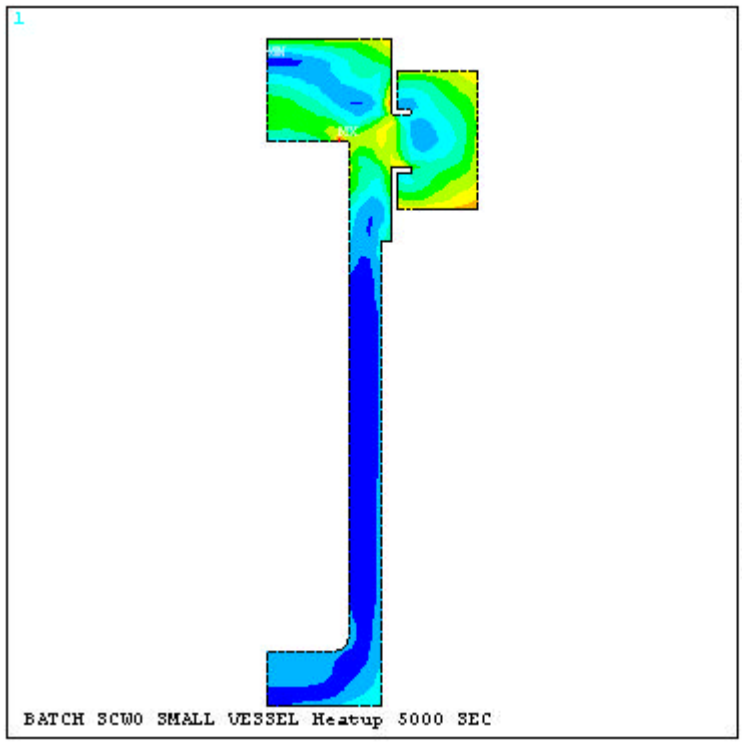

1
BATCH SCW0 SMALL VESSEL Heatup 600 SEC
ANSYS 5.5.1
MAY 22 2001
13:30:24
NODAL SOLUTION
STEP=2
SUB =1
TIME=2
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.028913
SMN =1415
SMX =37003
1415
5359
9323
13278
17232
21186
25141
29095
33049
37003

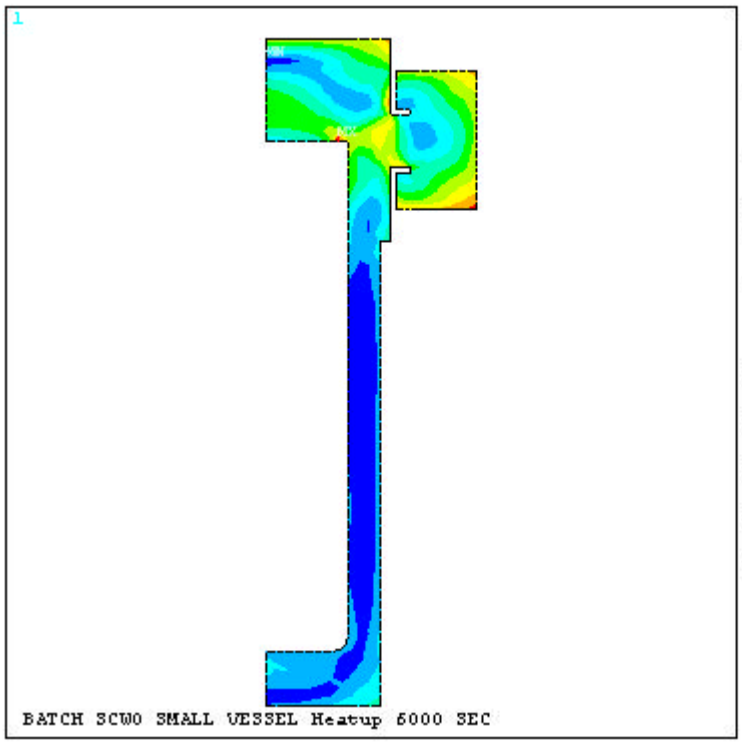

1
BATCH SCW0 SMALL VESSEL Heatup 1000 SEC
ANSYS 5.5.1
MAY 22 2001
13:30:46
NODAL SOLUTION
STEP=3
SUB =1
TIME=3
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.049496
SMN =431.744
SMX =45355
431.744
5423
10415
15406
20397
25389
30380
35372
40363
45355

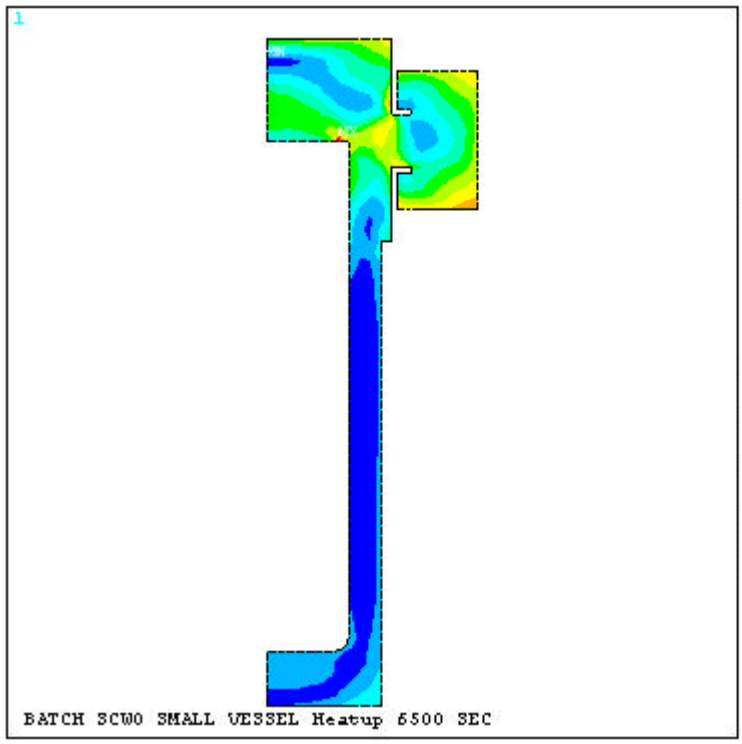

1
BATCH SCWO SMALL VESSEL Heatup 2000 SEC
ANSYS 5.5.1
MAY 22 2001
13:31:06
NODAL SOLUTION
STEP=4
SUB =1
TIME=4
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.090674
SMN =529.666
SMX =33951
529.666
4243
7957
11670
15384
19097
22811
26524
30237
33951

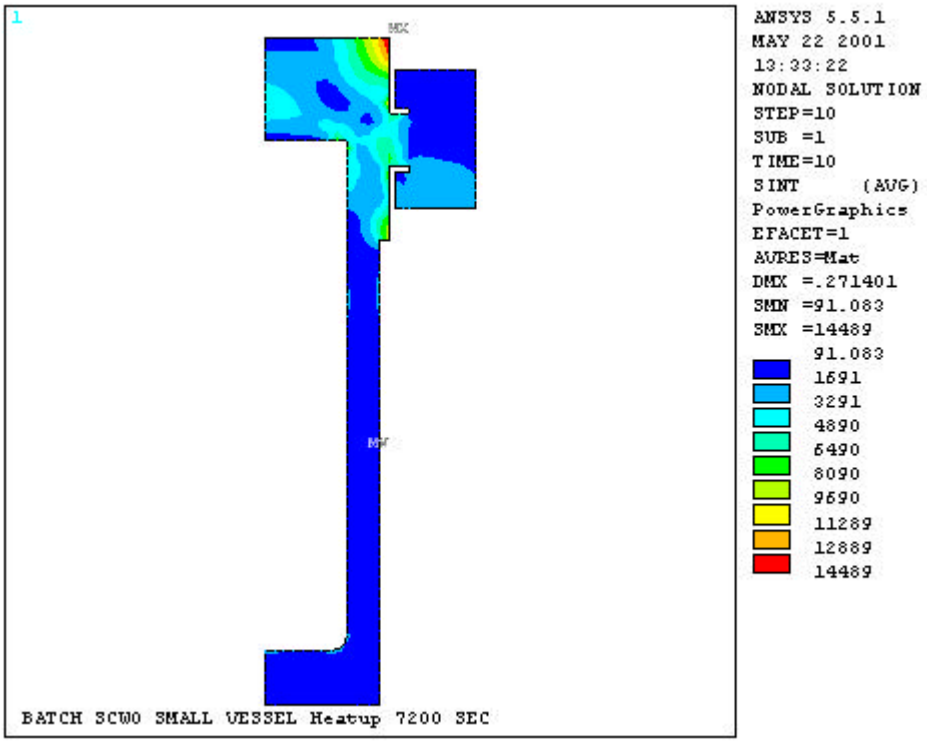

1
BATCH SCWO SMALL VESSEL Heatup 3000 SEC
ANSYS 5.5.1
MAY 22 2001
13:31:23
NODAL SOLUTION
STEP=5
SUB =1
TIME=5
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.13129
SMN =637.031
SMX =31918
637.031
4113
7588
11064
14540
18015
21491
24967
28442
31918


1
BATCH SCWO SMALL VESSEL Heatup 4000 SEC
ANSYS 5.5.1
MAY 22 2001
13:31:44
NODAL SOLUTION
STEP=6
SUB =1
TIME=6
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.1709
SMN =545.568
SMX =28354
545.568
3635
6725
9815
12905
15994
19084
22174
25264
28354


1
BATCH SCWO SMALL VESSEL Heatup 5000 SEC
ANSYS 5.5.1
MAY 22 2001
13:32:04
NODAL SOLUTION
STEP=7
SUB =1
TIME=7
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.208937
SMN =388.794
SMX =25649
388.794
3195
6002
8809
11615
14422
17229
20035
22842
25649

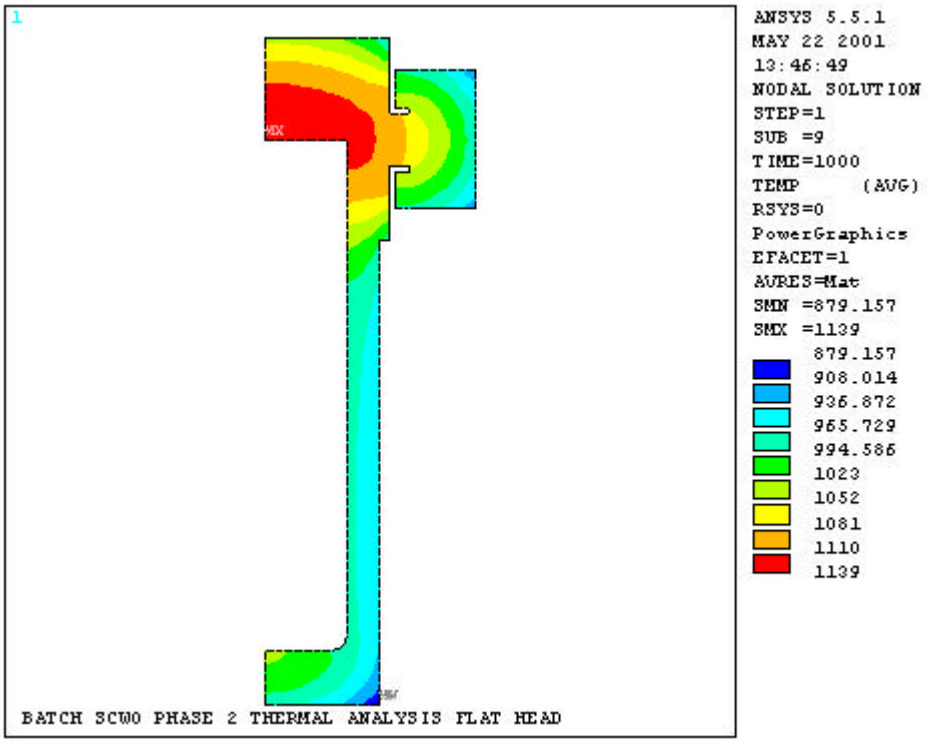

1
ANSYS 5.5.1
MAY 22 2001
13:32:25
NODAL SOLUTION
STEP=8
SUB =1
TIME=8
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.246229
SMN =84.254
SMX =24257
84.254
2770
5456
8142
10828
13513
16199
18885
21571
24257
BATCH SCWO SMALL VESSEL Heatup 6000 SEC


1
ANSYS 5.5.1
MAY 22 2001
13:32:52
NODAL SOLUTION
STEP=9
SUB =1
TIME=9
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.265908
SMN =326.606
SMX =25309
326.606
3102
5878
8654
11430
14206
16982
19758
22534
25309
BATCH SCWO SMALL VESSEL Heatup 6500 SEC

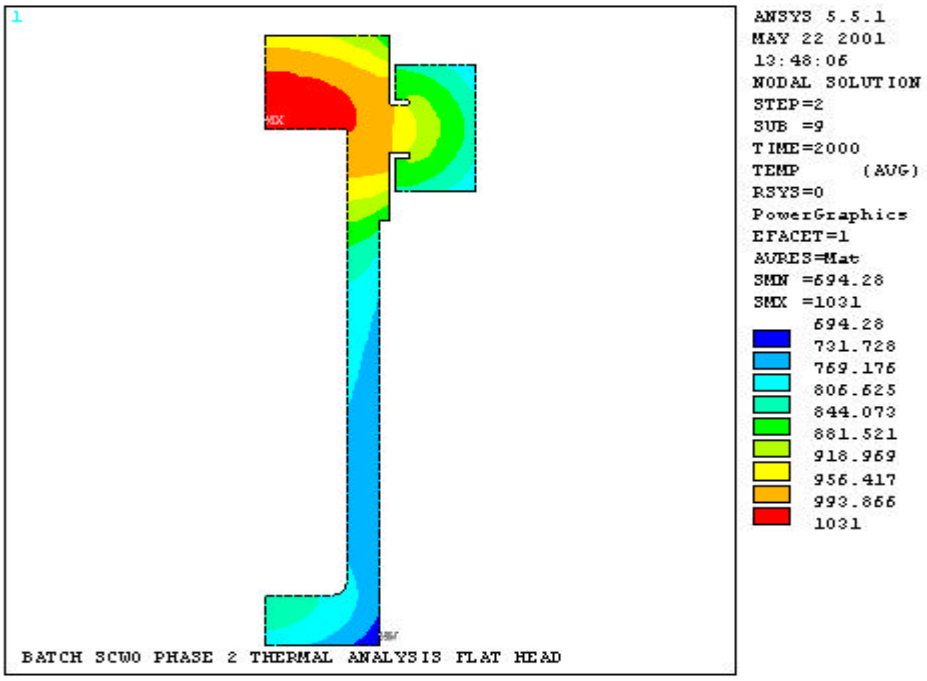

1
MX
MN
BATCH SCW0 SMALL VESSEL Heatup 7200 SEC
ANSYS 5.5.1
MAY 22 2001
13:33:22
NODAL SOLUTION
STEP=10
SUB =1
TIME=10
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.271401
SMN =91.083
SMX =14489
91.083
1691
3291
4890
6490
8090
9690
11289
12889
14489

7.8 Small Vessel Thermal Contour Plots – Cooldown Transient

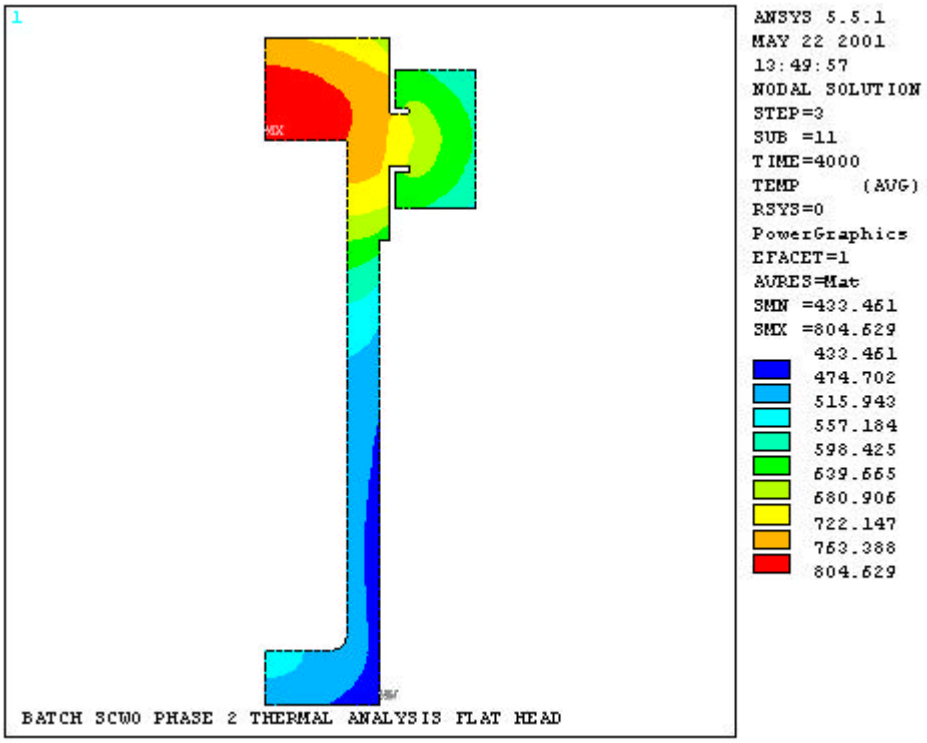
The temperature contour plots contained in this section are for selected time steps in the ANSYS solution for the small vessel cooldown transient. The forced convection film coefficient derived in Section 7.4 is applied uniformly to the outer surfaces of the model with a bulk air temperature of 70F. The model is initially set to a uniform 1200F. As can be seen in the plots the model is between 77F and 1131F at 18000 sec.



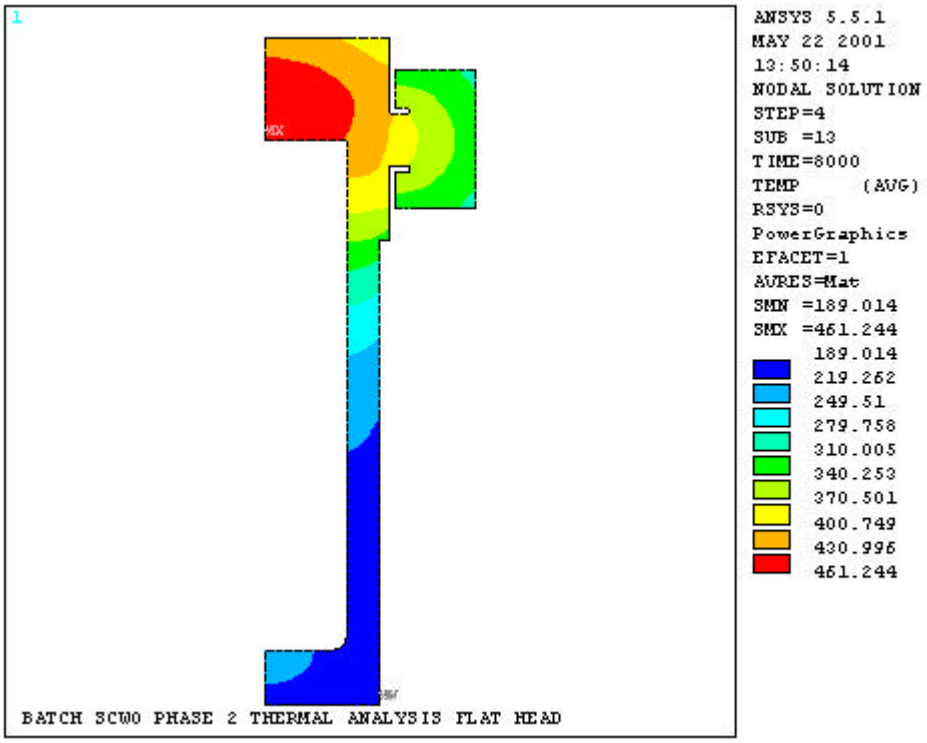
Batch SCWO Small Vessel 1000 sec



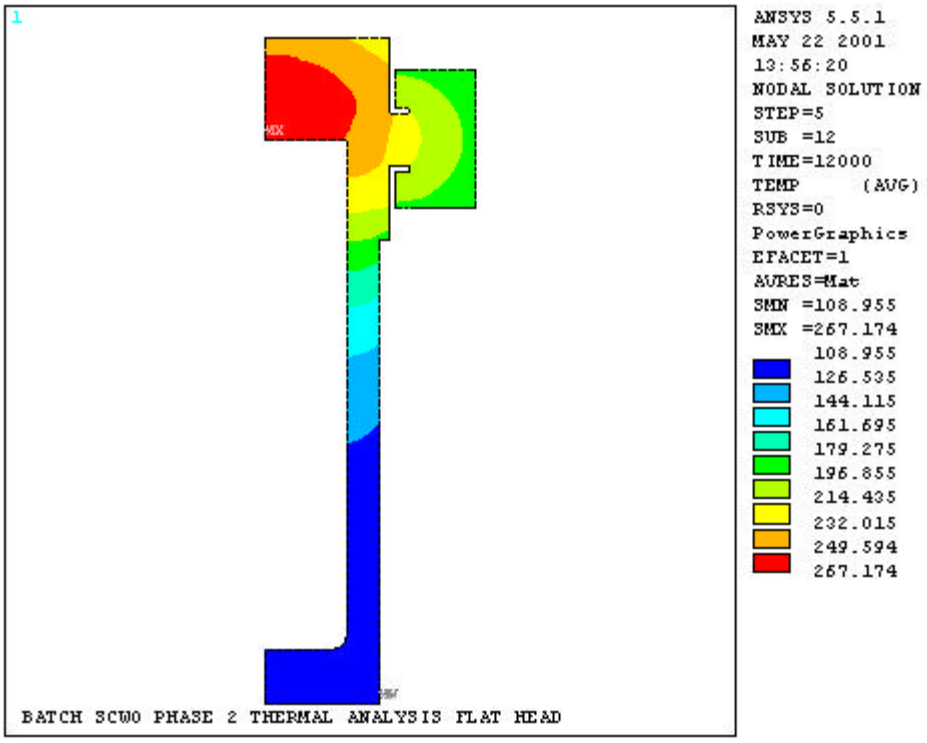
Batch SCWO Small Vessel 2000 sec



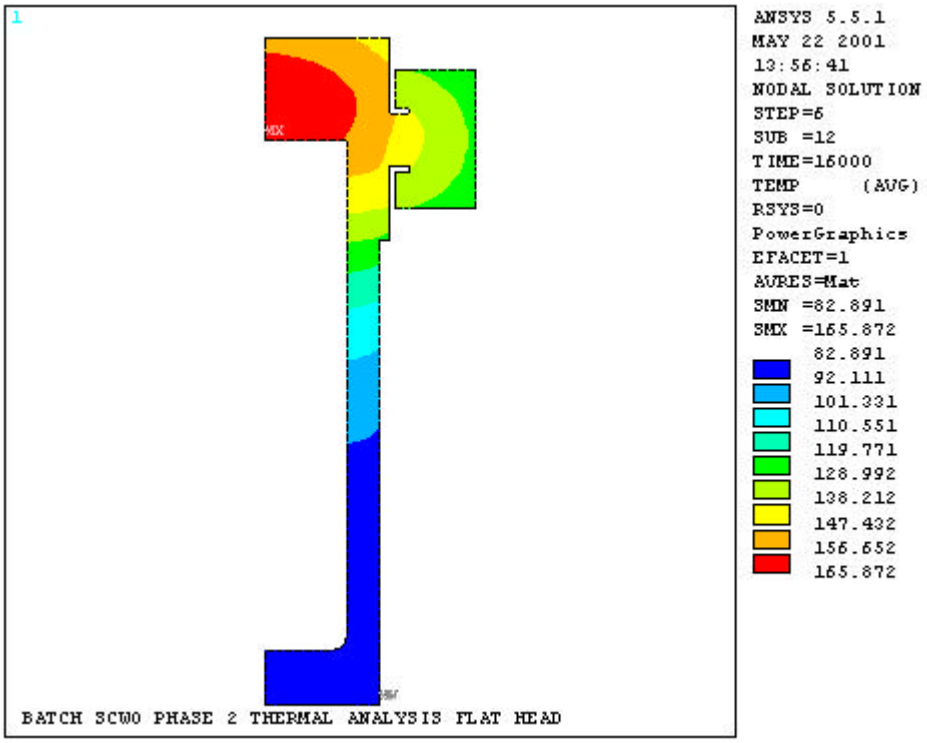
Batch SCWO Small Vessel 4000 sec



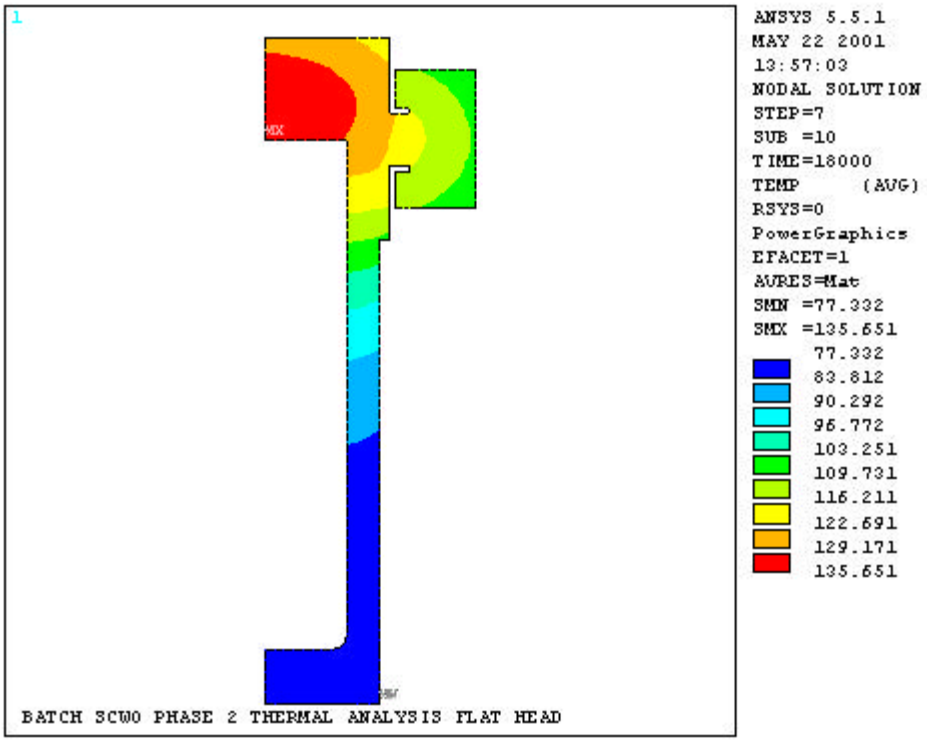
Batch SCWO Small Vessel 8000 sec



Batch SCWO Small Vessel 12,000 sec



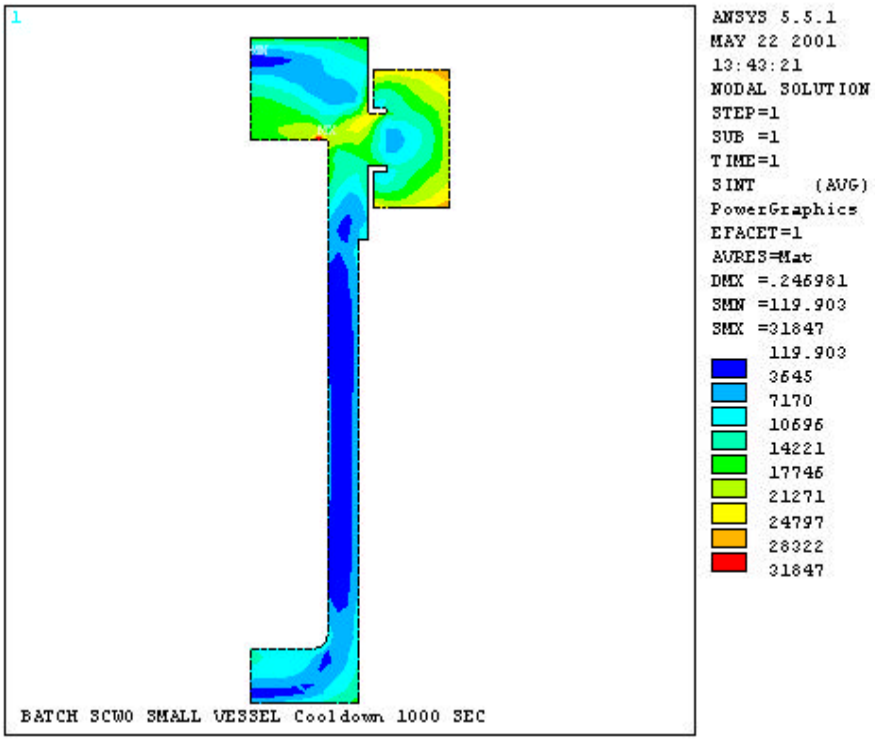
Batch SCWO Small Vessel 16,000 sec

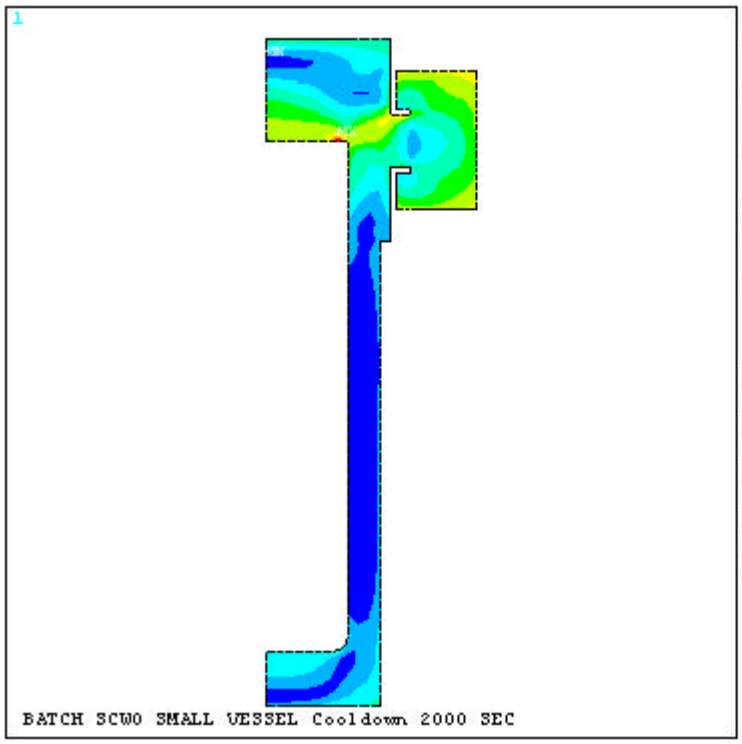


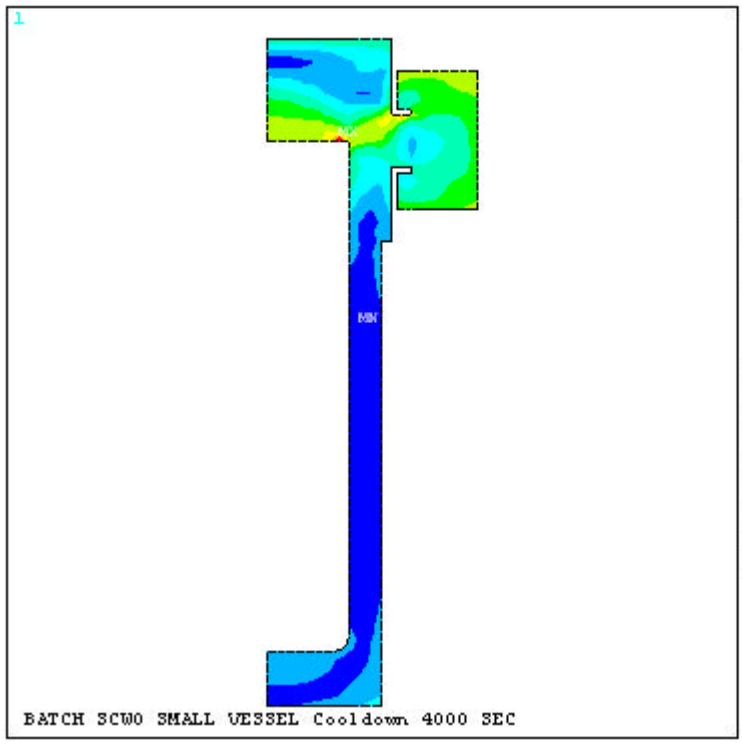
Batch SCWO Small Vessel 18,000 sec

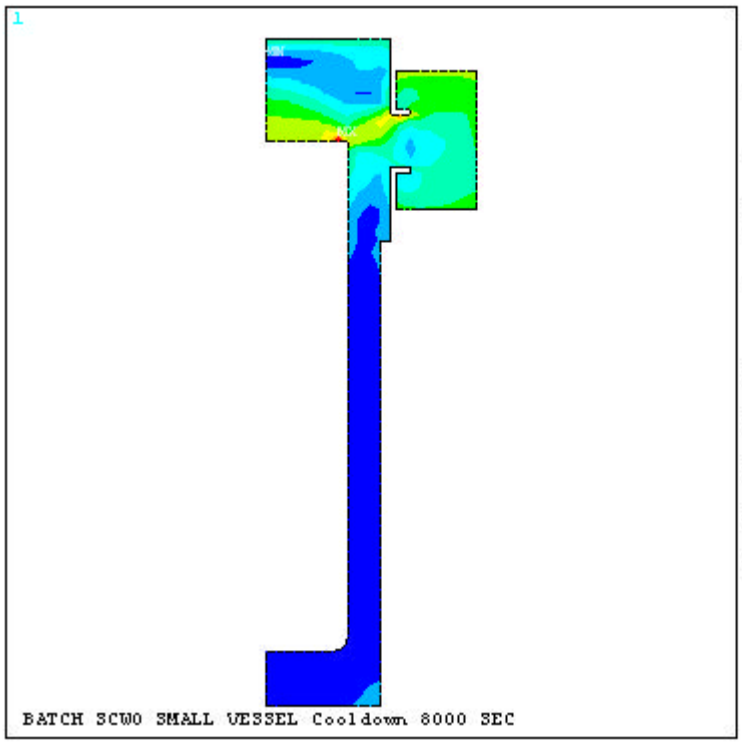
7.9 Small Vessel Stress Contour Plots – Cooldown Transient

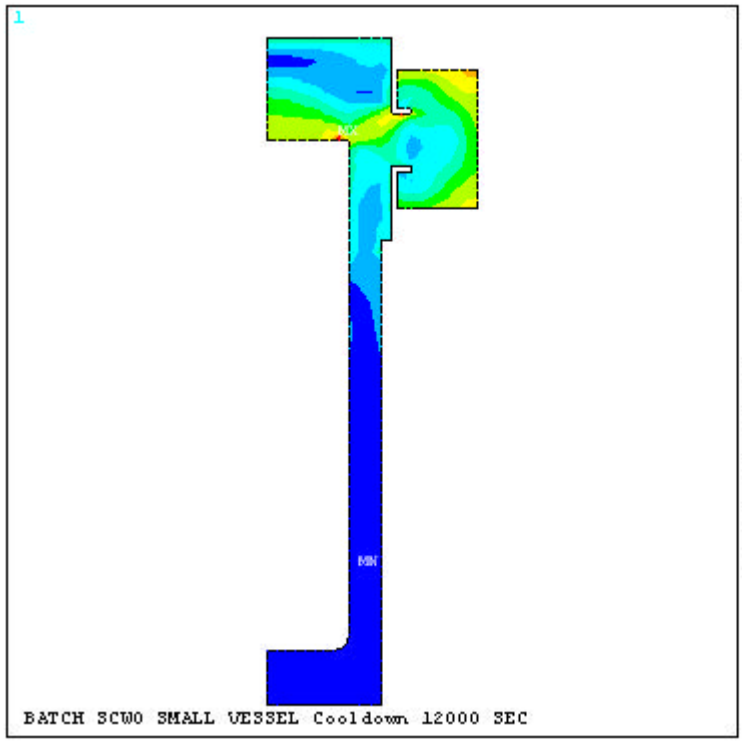
The stress intensity contour plots contained in this section are calculated for the temperature distribution corresponding to the selected time steps in the ANSYS solution for the small vessel cool down transient. The maximum stress intensity is located on the inside surface of the head, occurs at 4000 sec. and is equal to 38547psi.

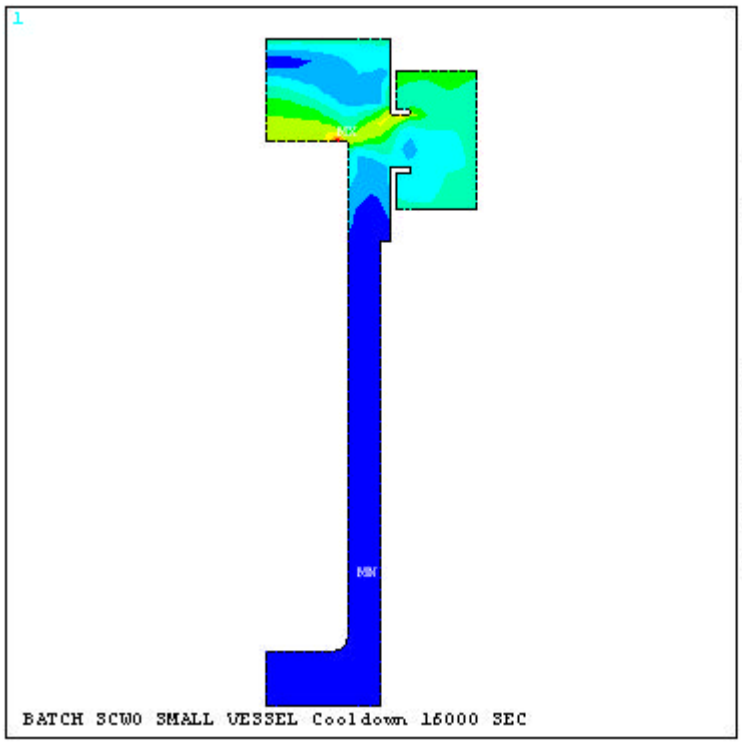


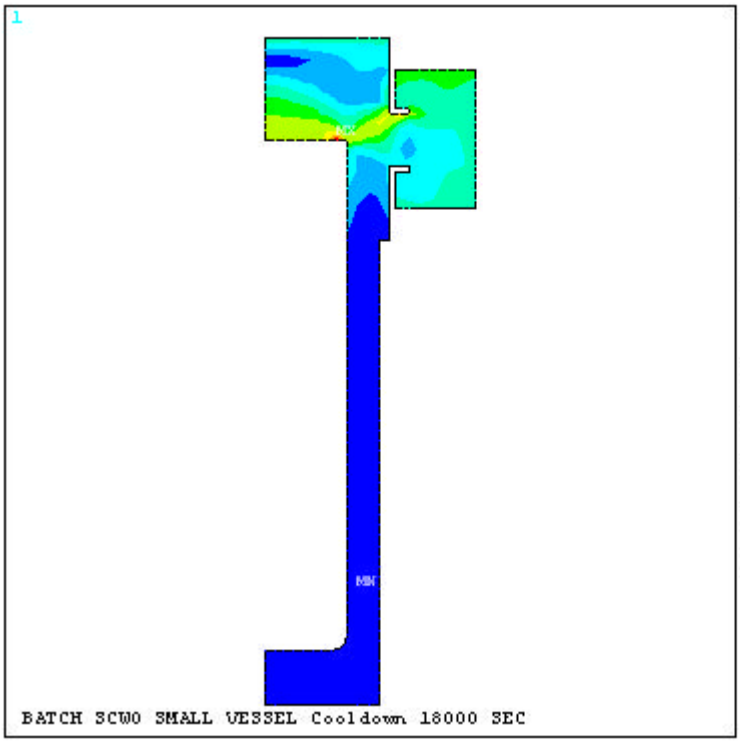

1
MN
MX
BATCH SCW0 SMALL VESSEL Cooldown 2000 SEC
ANSYS 5.5.1
MAY 22 2001
13:43:44
NODAL SOLUTION
STEP=2
SUB =1
TIME=2
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.202214
SMN =309.361
SMX =37108
309.361
4398
8487
12576
16664
20753
24842
28931
33019
37108


1
MN
MX
BATCH SCW0 SMALL VESSEL Cooldown 4000 SEC
ANSYS 5.5.1
MAY 22 2001
13:44:02
NODAL SOLUTION
STEP=3
SUB =1
TIME=3
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.134282
SMN =167.328
SMX =38647
167.328
4443
8718
12994
17269
21545
25821
30096
34372
38647


1
MX
MN
BATCH SCW0 SMALL VESSEL Cooldown 8000 SEC
ANSYS 5.5.1
MAY 22 2001
13:44:25
NODAL SOLUTION
STEP=4
SUB =1
TIME=4
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.061958
SMN =140.716
SMX =25958
140.716
3009
5878
8747
11615
14484
17352
20221
23090
25958

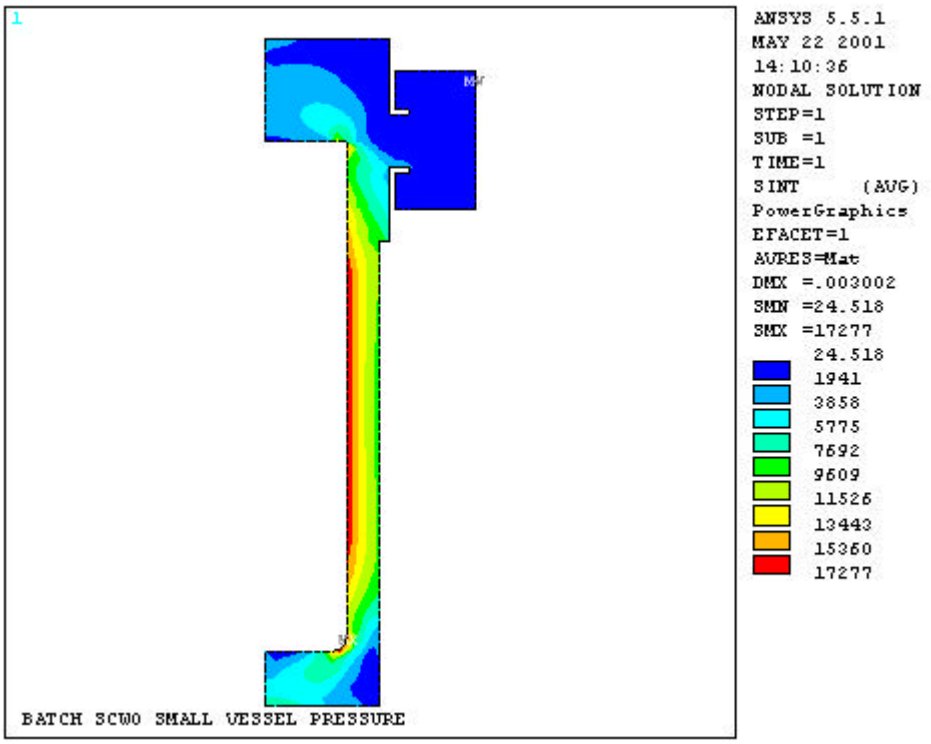

1
MX
MN
BATCH SCW0 SMALL VESSEL Cooldown 12000 SEC
ANSYS 5.5.1
MAY 22 2001
13:44:52
NODAL SOLUTION
STEP=5
SUB =1
TIME=5
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.024905
SMN =62.084
SMX =14246
62.084
1638
3214
4790
6366
7942
9518
11094
12670
14246


1
ANSYS 5.5.1
MAY 22 2001
13:45:17
NODAL SOLUTION
STEP=6
SUB =1
TIME=6
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.007998
SMN =8.96
SMX =11086
8.96
1240
2470
3701
4932
6163
7394
8624
9855
11086
MN
MX
BATCH SCWO SMALL VESSEL Cooldown 16000 SEC


1
ANSYS 5.5.1
MAY 22 2001
13:45:40
NODAL SOLUTION
STEP=7
SUB =1
TIME=7
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.004088
SMN =5.511
SMX =5975
5.511
668.835
1332
1995
2659
3322
3985
4649
5312
5975
MN
MX
BATCH SCWO SMALL VESSEL Cooldown 18000 SEC

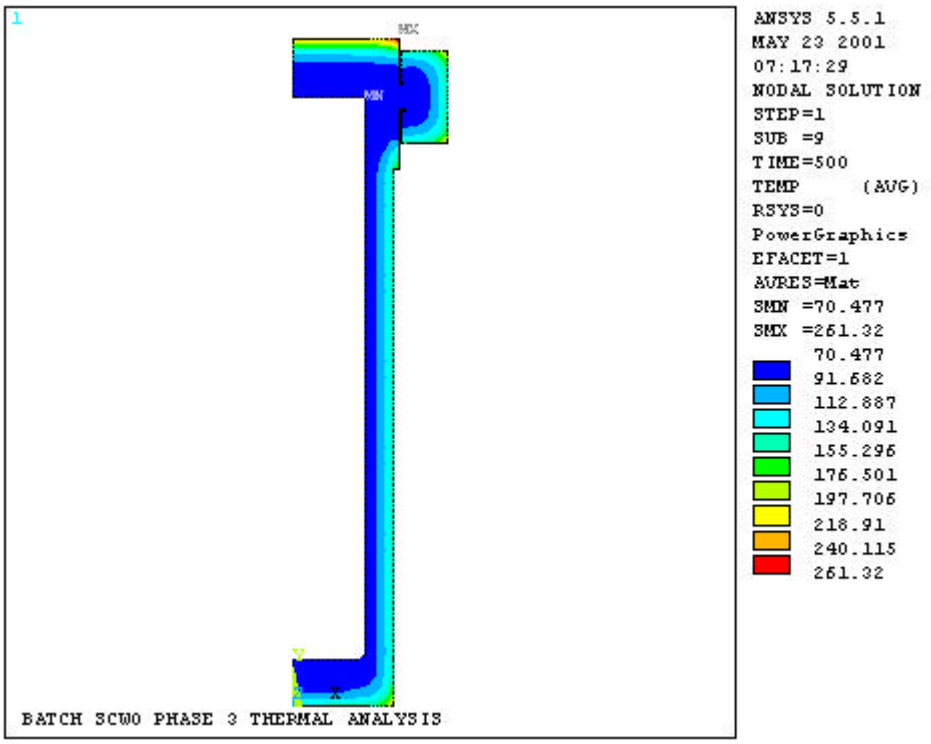
7.10 Small Vessel Stress Contour Plots – Pressure

A pressure load of 4000 psi is applied to the inner surfaces of the model and the resulting stress intensity contours are shown in the plot below. Maximum pressure stress occurs at the shell to bottom head fillet.

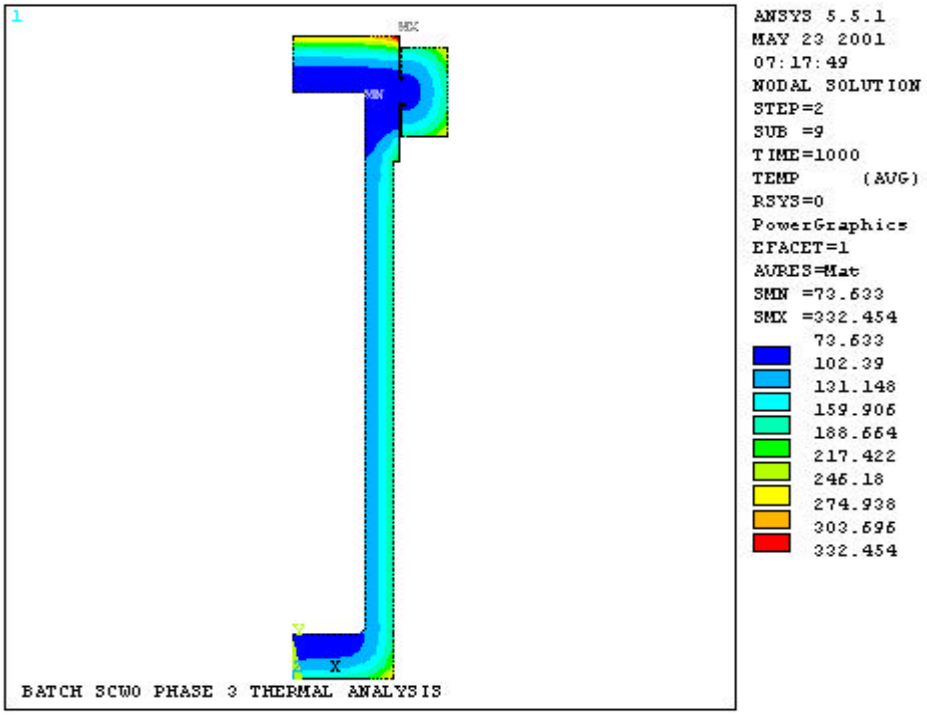


7.11 Large Vessel Thermal Contour Plots – Heatup Transient

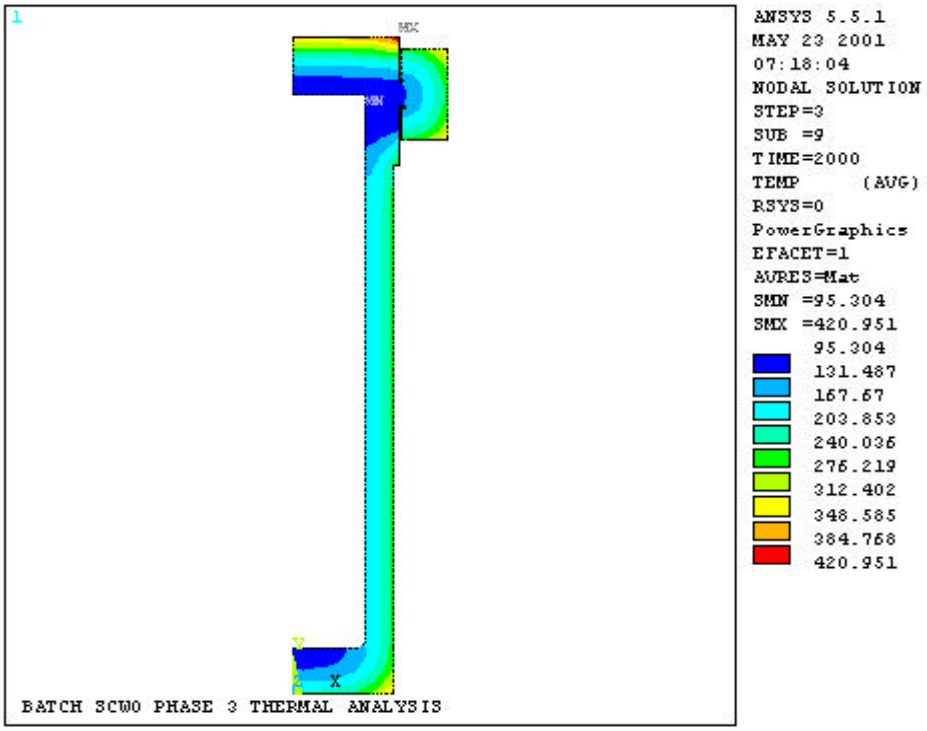
The temperature contour plots contained in this section are for selected time steps in the ANSYS solution for the large vessel heat-up transient. Heat flux input loading varies between 7 watts/sq. in along the vessel shell and 15 watts/sq. in at the heads. The model is initially at 70°F and the heat flux is applied as a constant value until 18000 sec where it is removed. The model is allowed to equilibrate until 19800 sec. As can be seen in the plots the model is between 971°F and 1131°F at 19800 sec.



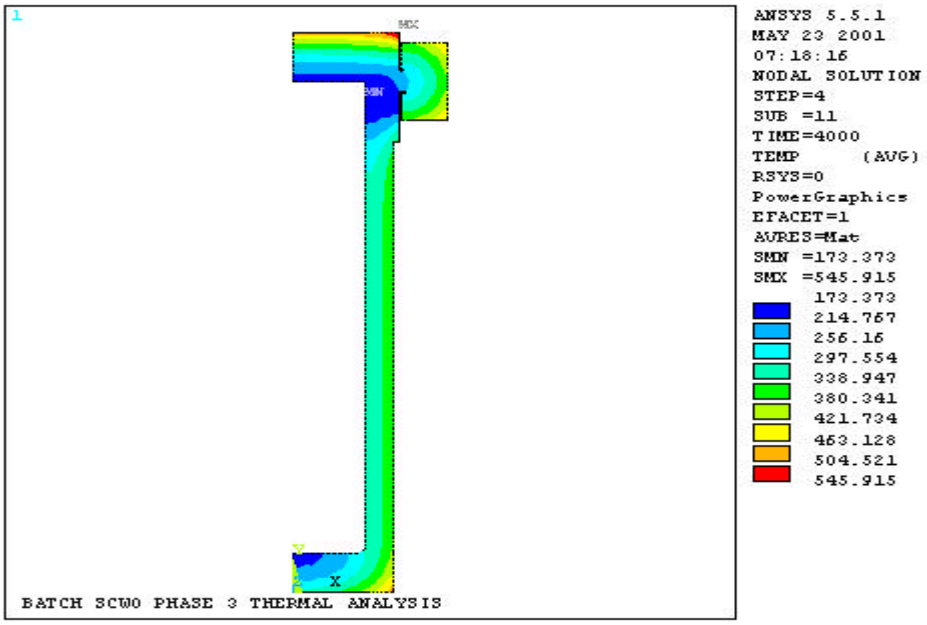
Batch SCWO Large Vessel 500 sec



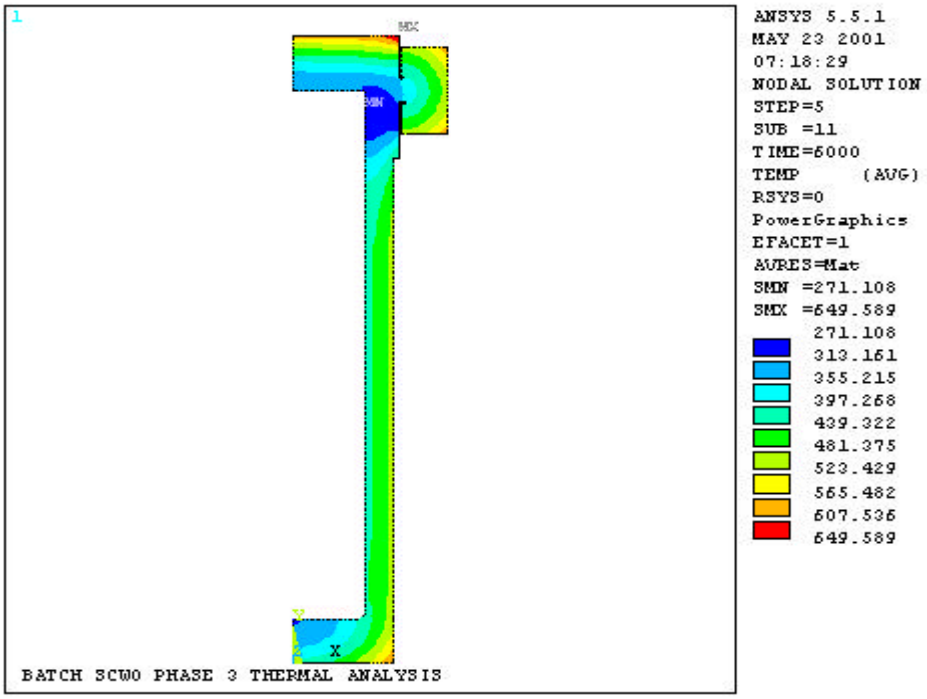
Batch SCWO Large Vessel 1000 sec



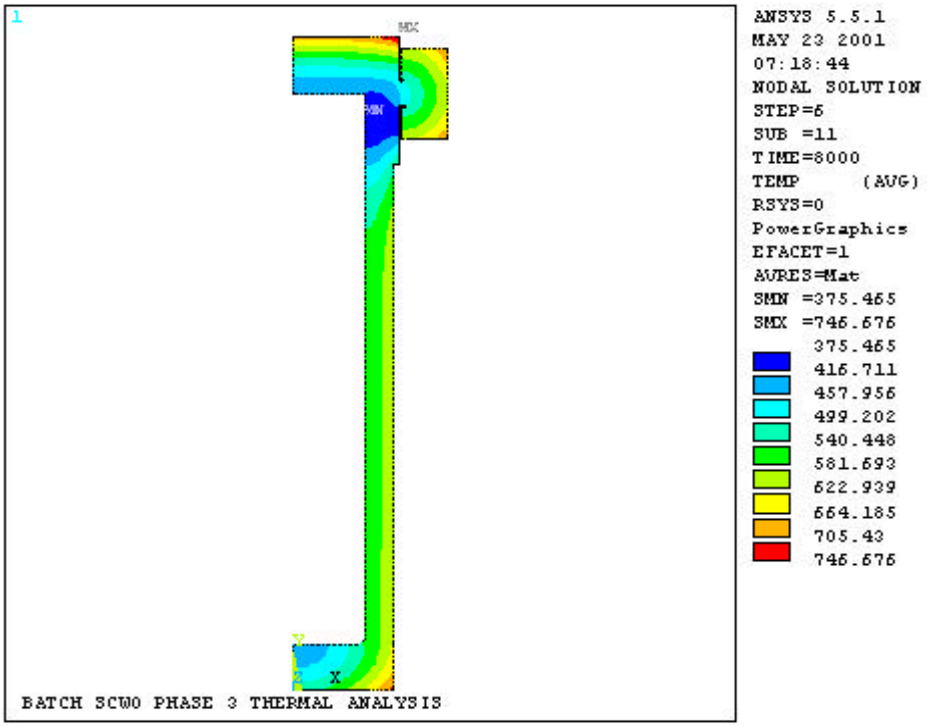
Batch SCWO Large Vessel 2000 sec



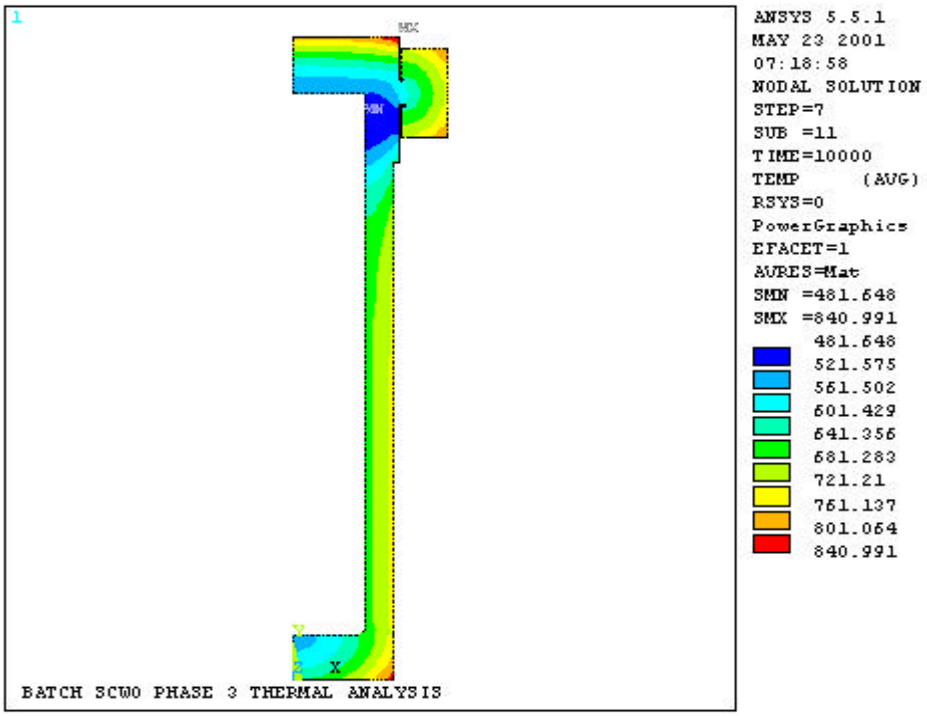
Batch SCWO Large Vessel 4000 sec



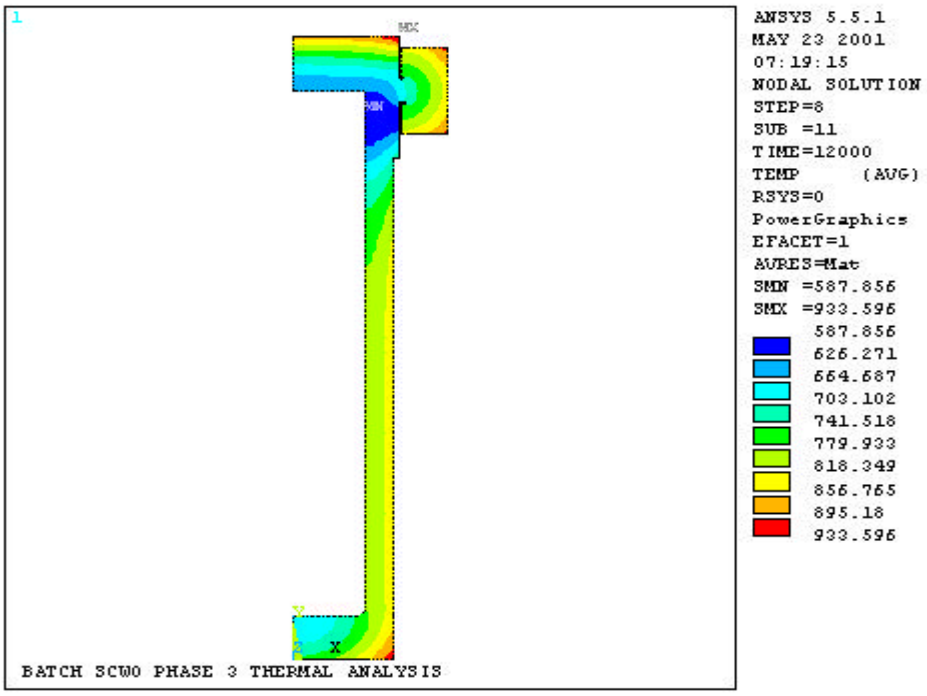
Batch SCWO Large Vessel 6000 sec



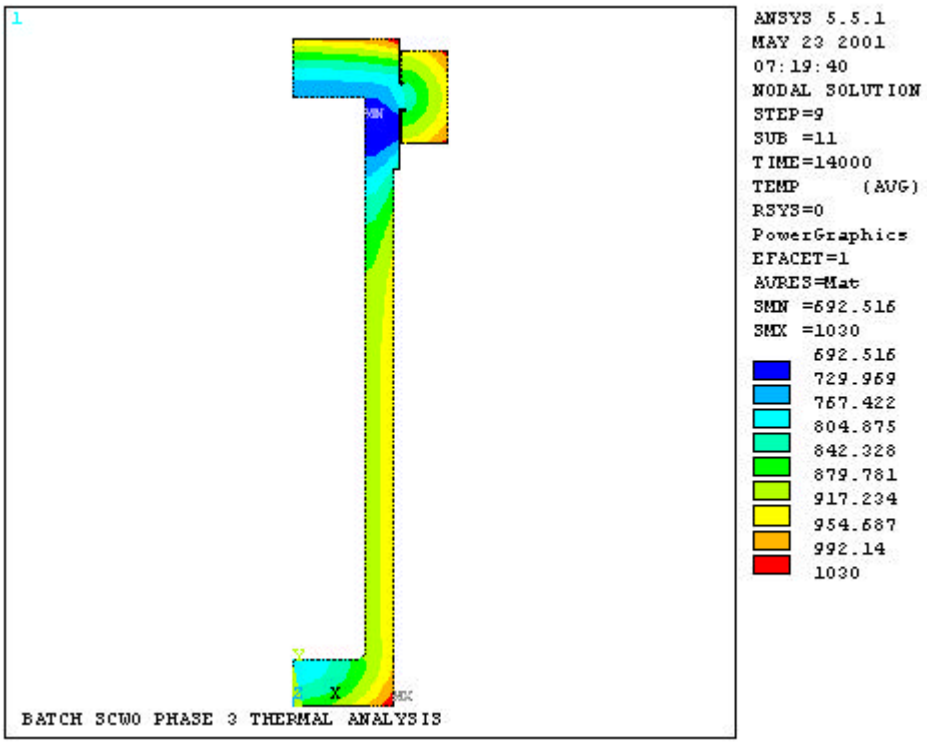
Batch SCWO Large Vessel 8000 sec



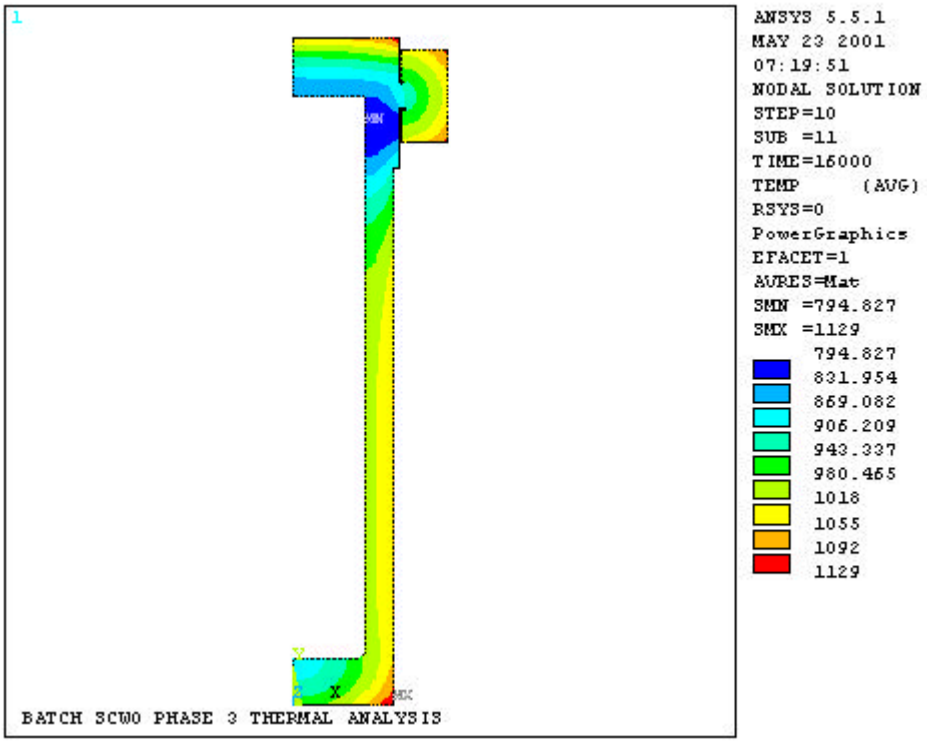
Batch SCWO Large Vessel 10,000 sec



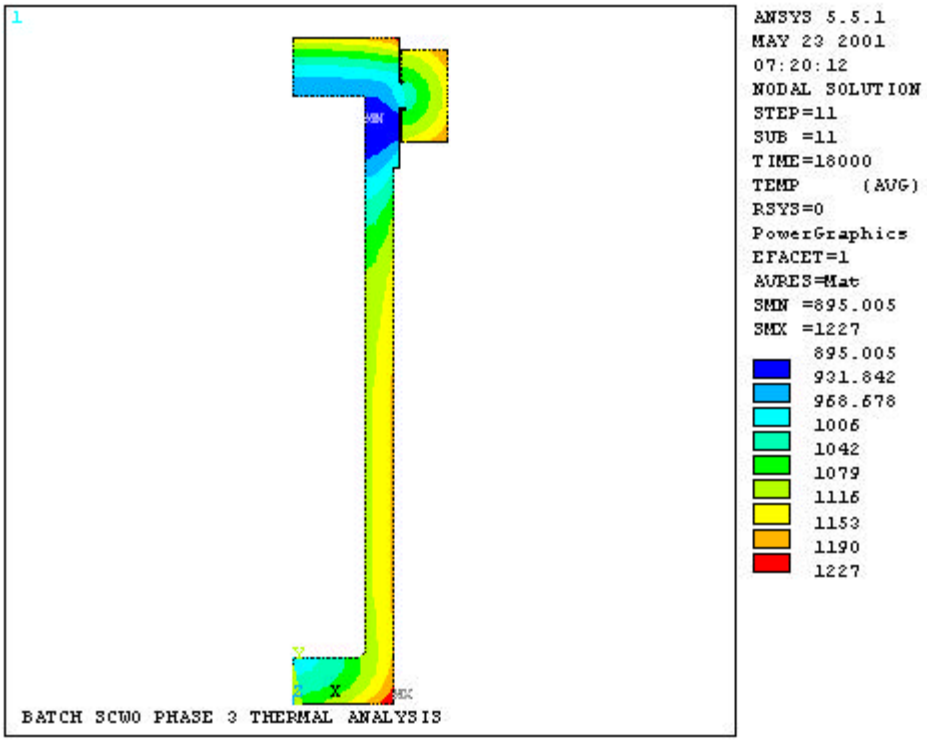
Batch SCWO Large Vessel 12,000 sec



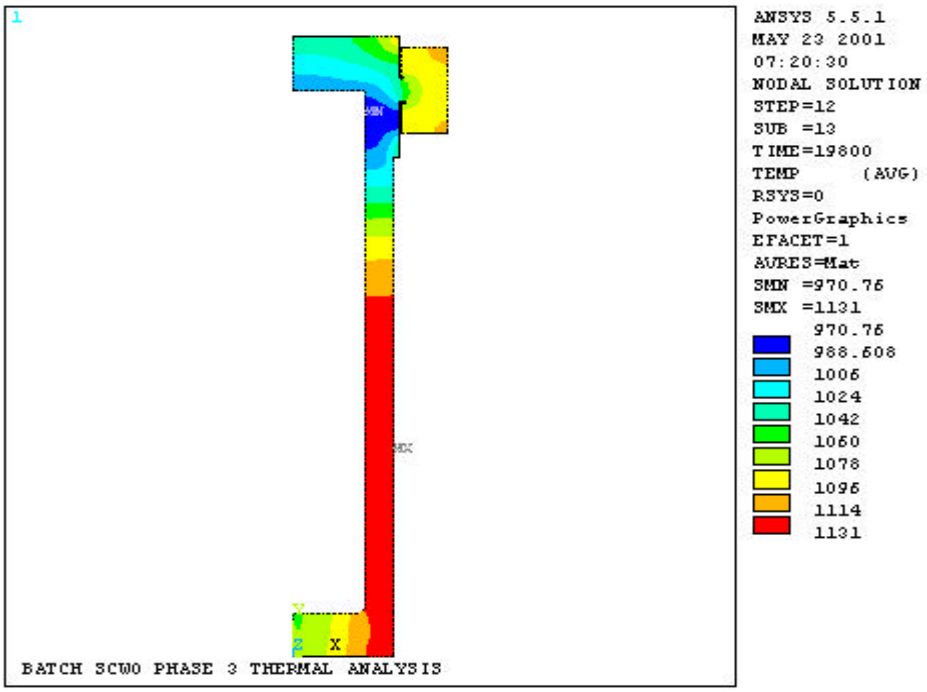
Batch SCWO Large Vessel 14,000 sec



Batch SCWO Large Vessel 16,000 sec



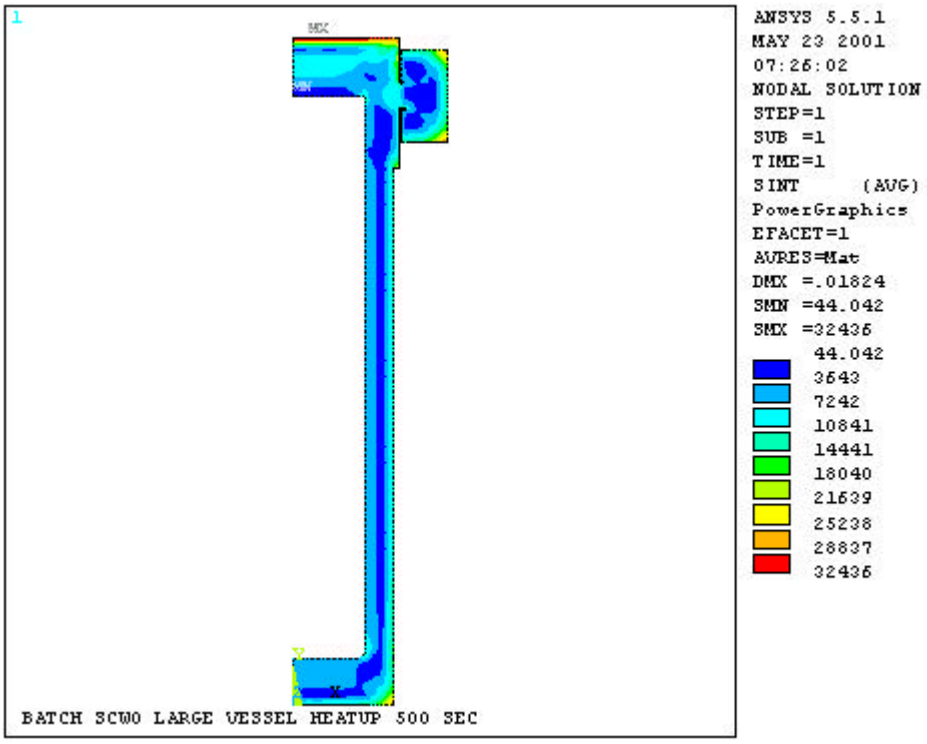
Batch SCWO Large Vessel 18,000 sec

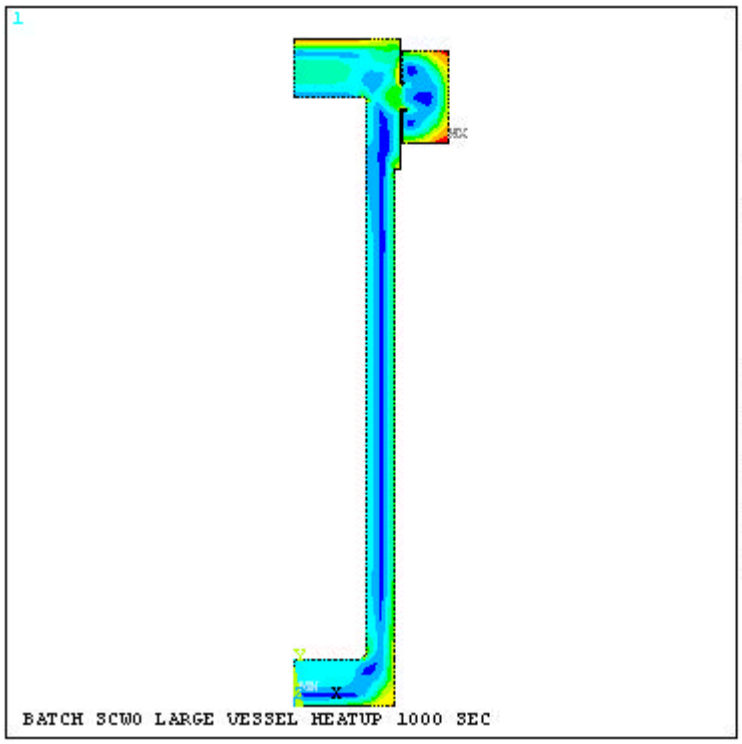


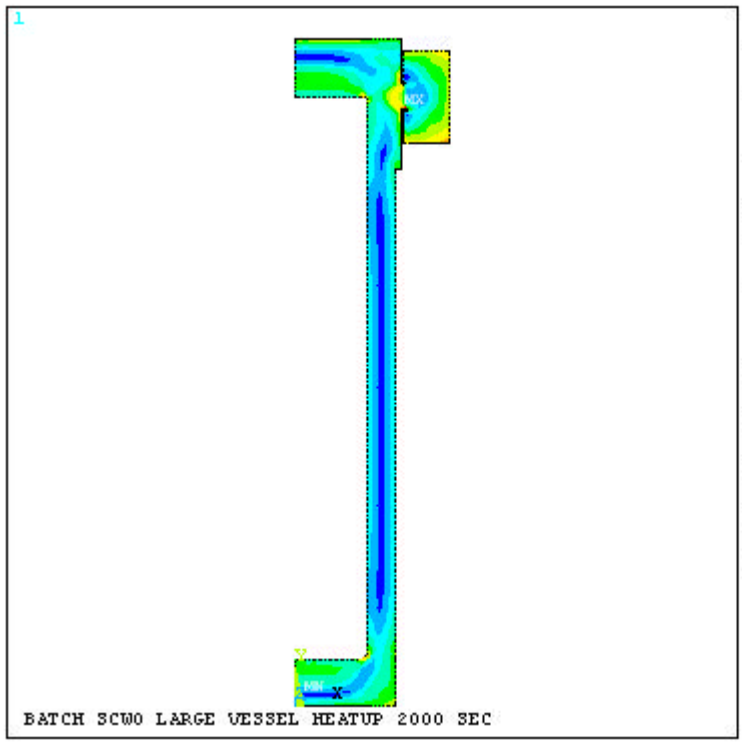
Batch SCWO Large Vessel 19,800 sec

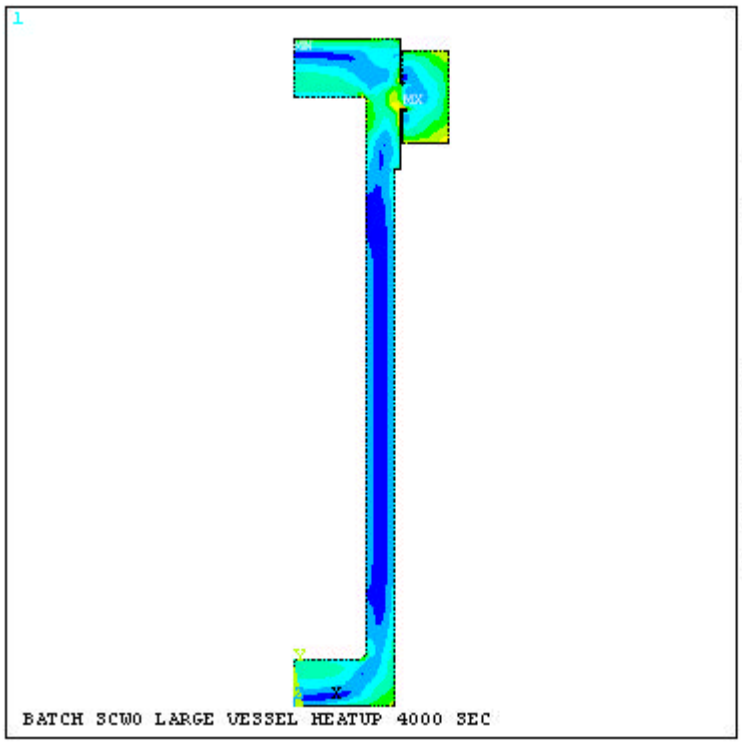
7.12 Large Vessel Stress Contour Plots – Heatup Transient

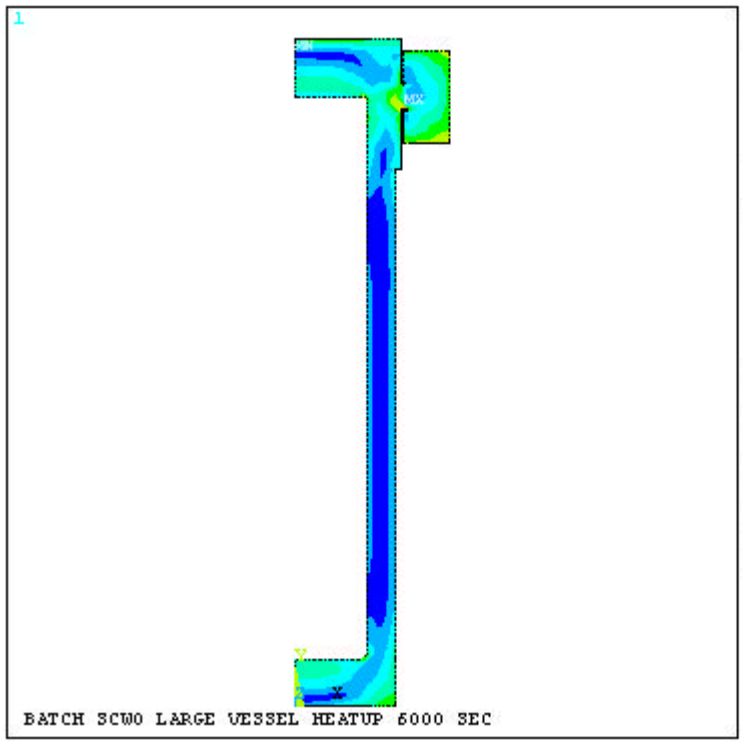
The stress intensity contour plots contained in this section are calculated for the temperature distribution corresponding to the selected time steps in the ANSYS solution for the large vessel heat-up transient. The maximum stress intensity is located in the clamp/flange, occurs at 10000 sec. and is equal to 63875psi. Note that results presented for the clamp are only for informational purposes as the model is only relevant for the shell/and lower head.

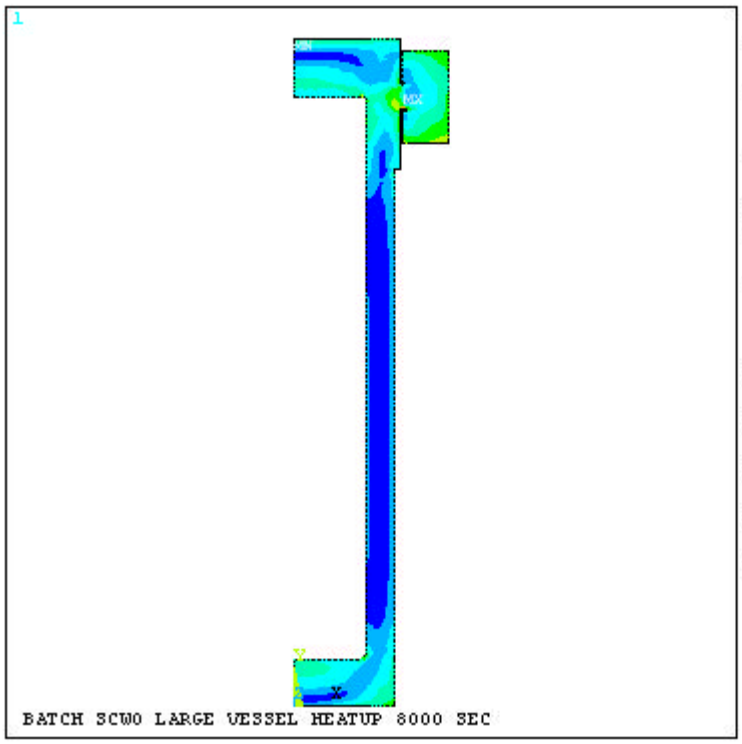


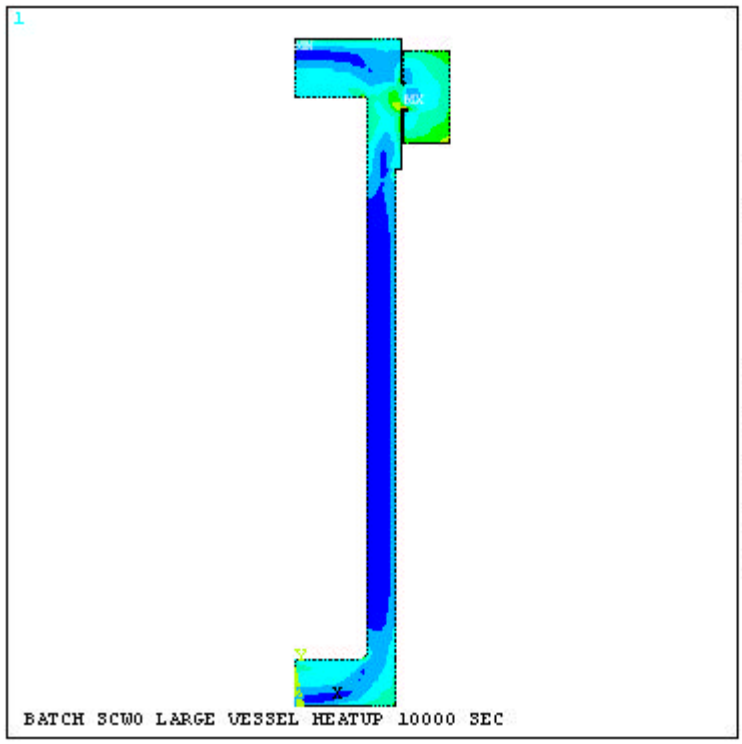

1
ANSYS 5.5.1
MAY 23 2001
07:26:18
NODAL SOLUTION
STEP=2
SUB =1
TIME=2
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.046514
SMN =80.543
SMX =40853
80.543
4611
9141
13671
18202
22732
27262
31793
36323
40853
BATCH SCWO LARGE VESSEL HEATUP 1000 SEC

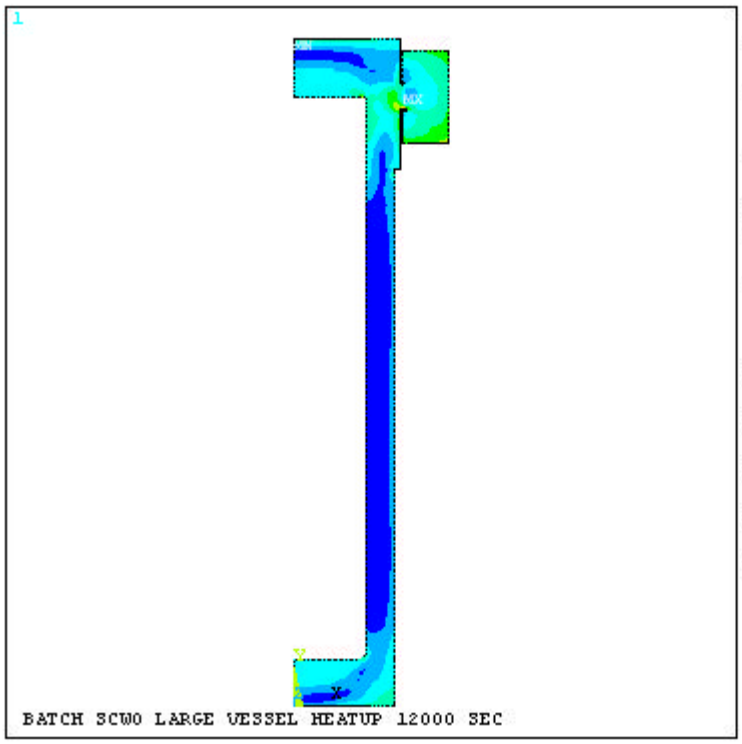

1
ANSYS 5.5.1
MAY 23 2001
07:26:32
NODAL SOLUTION
STEP=3
SUB =1
TIME=3
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.113627
SMN =569.632
SMX =50770
569.632
6147
11725
17303
22881
28459
34037
39614
45192
50770
BATCH SCWO LARGE VESSEL HEATUP 2000 SEC

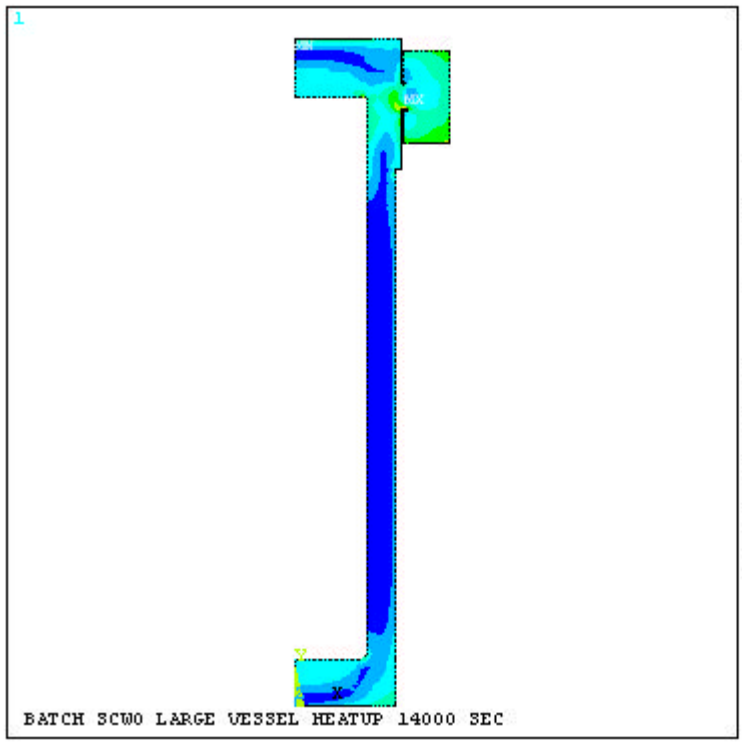

1
BATCH SCW0 LARGE VESSEL HEATUP 4000 SEC
ANSYS 5.5.1
MAY 23 2001
07:26:50
NODAL SOLUTION
STEP=4
SUB =1
TIME=4
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.204316
SMN =153.86
SMX =54776
153.86
6223
12292
18361
24431
30500
36569
42638
48707
54776

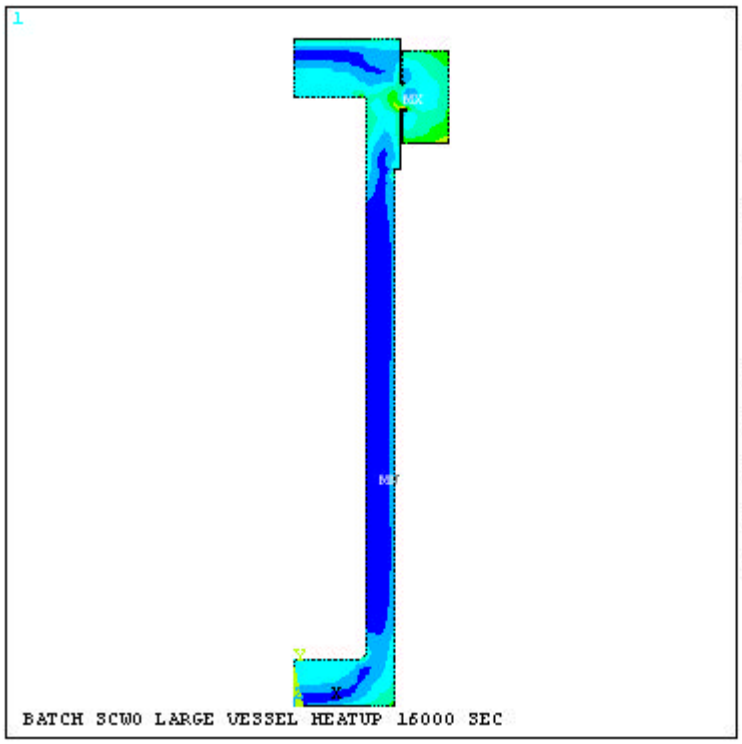

1
BATCH SCW0 LARGE VESSEL HEATUP 6000 SEC
ANSYS 5.5.1
MAY 23 2001
07:27:13
NODAL SOLUTION
STEP=5
SUB =1
TIME=5
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.290474
SMN =38.988
SMX =60027
38.988
6704
13370
20035
26700
33366
40031
46697
53362
60027

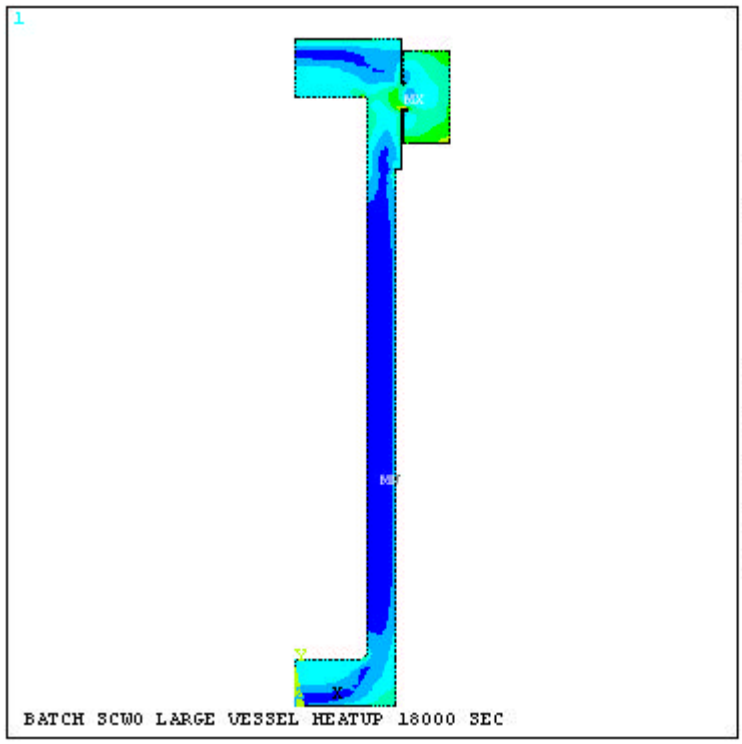

1
BATCH SCW0 LARGE VESSEL HEATUP 8000 SEC
ANSYS 5.5.1
MAY 23 2001
07:27:33
NODAL SOLUTION
STEP=6
SUB =1
TIME=6
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.376688
SMN =90.832
SMX =63459
90.832
7132
14173
21214
28255
35295
42336
49377
56418
63459

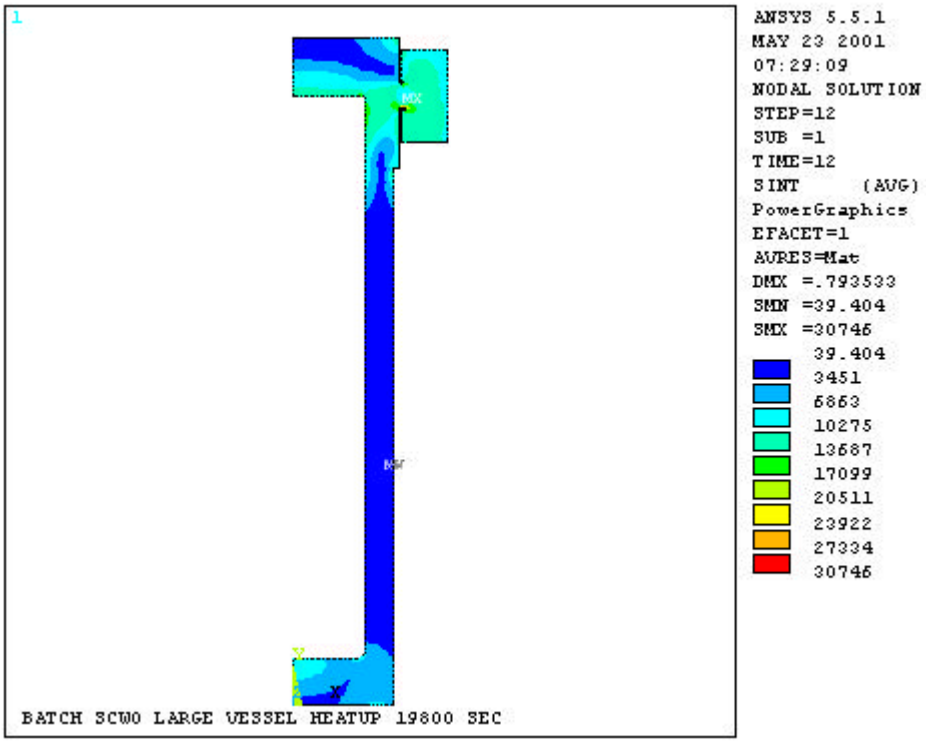

1
BATCH SCW0 LARGE VESSEL HEATUP 10000 SEC
ANSYS 5.5.1
MAY 23 2001
07:27:46
NODAL SOLUTION
STEP=7
SUB =1
TIME=7
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.460814
SMN =196.949
SMX =63876
196.949
7272
14348
21423
28499
35574
42649
49725
56800
63876


1
ANSYS 5.5.1
MAY 23 2001
07:28:07
NODAL SOLUTION
STEP=8
SUB =1
TIME=8
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.54299
SMN =322.137
SMX =61599
322.137
7131
13939
20748
27556
34365
41173
47982
54790
61599
BATCH SCWO LARGE VESSEL HEATUP 12000 SEC


1
ANSYS 5.5.1
MAY 23 2001
07:28:26
NODAL SOLUTION
STEP=9
SUB =1
TIME=9
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.622603
SMN =530.278
SMX =59453
530.278
7077
13624
20171
26718
33265
39812
46359
52906
59453
BATCH SCWO LARGE VESSEL HEATUP 14000 SEC

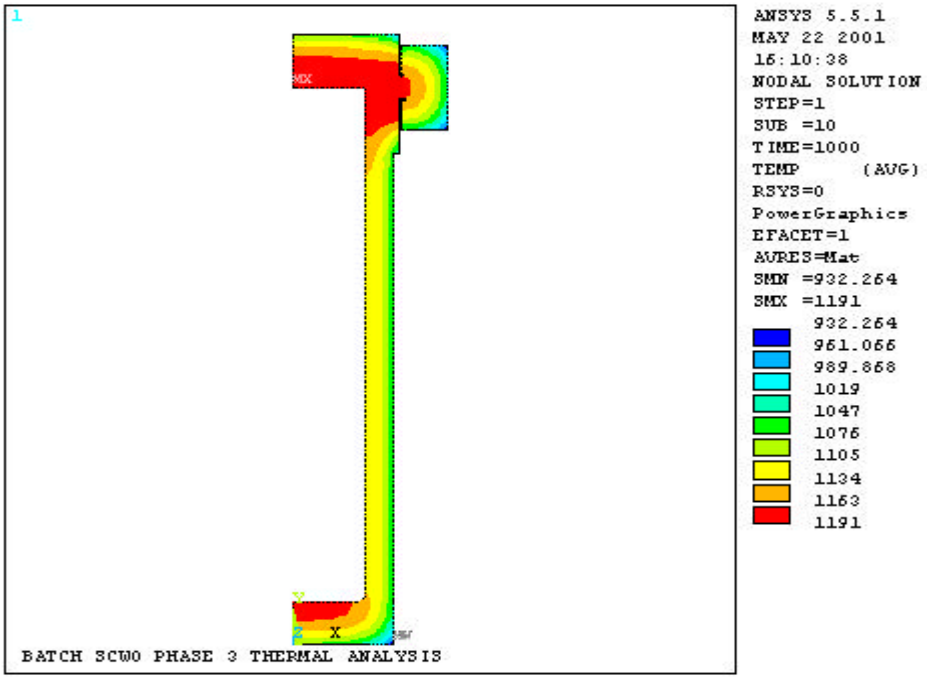

1
MX
MN
BATCH SCWO LARGE VESSEL HEATUP 16000 SEC
ANSYS 5.5.1
MAY 23 2001
07:28:42
NODAL SOLUTION
STEP=10
SUB =1
TIME=10
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.702587
SMN =864.249
SMX =57306
864.249
7136
13407
19678
25950
32221
38492
44764
51035
57306


1
MX
MN
BATCH SCWO LARGE VESSEL HEATUP 18000 SEC
ANSYS 5.5.1
MAY 23 2001
07:28:54
NODAL SOLUTION
STEP=11
SUB =1
TIME=11
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.787854
SMN =833.903
SMX =58735
833.903
7267
13701
20134
26568
33001
39435
45868
52301
58735

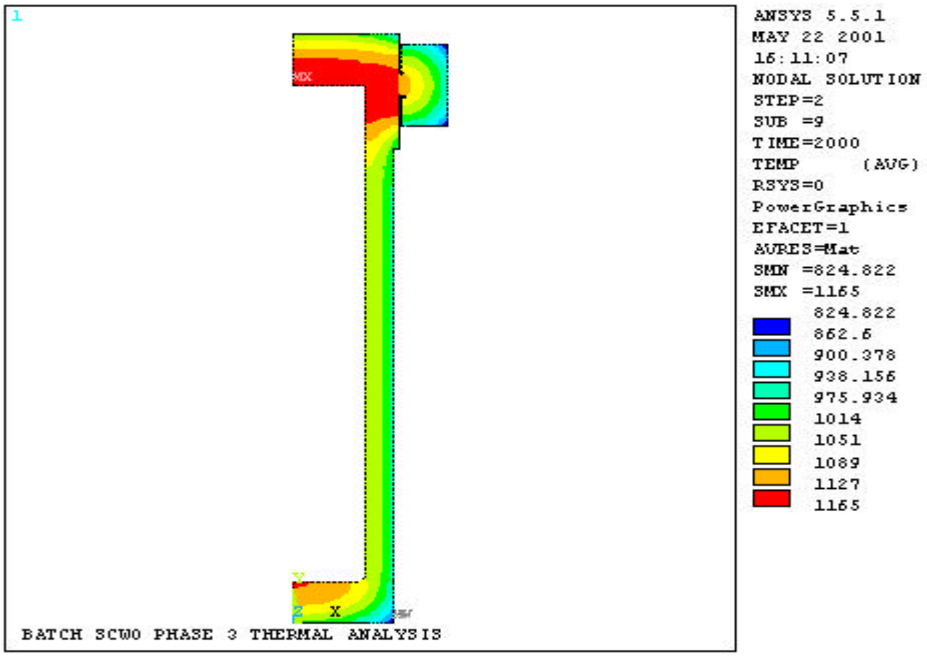

1
MX
MN
ANSYS 5.5.1
MAY 23 2001
07:29:09
NODAL SOLUTION
STEP=12
SUB =1
TIME=12
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.793533
SMN =39.404
SMX =30746
39.404
3451
6863
10275
13687
17099
20511
23922
27334
30746
BATCH SCWO LARGE VESSEL HEATUP 19800 SEC

7.13 Large Vessel Thermal Contour Plots – Cooldown Transient

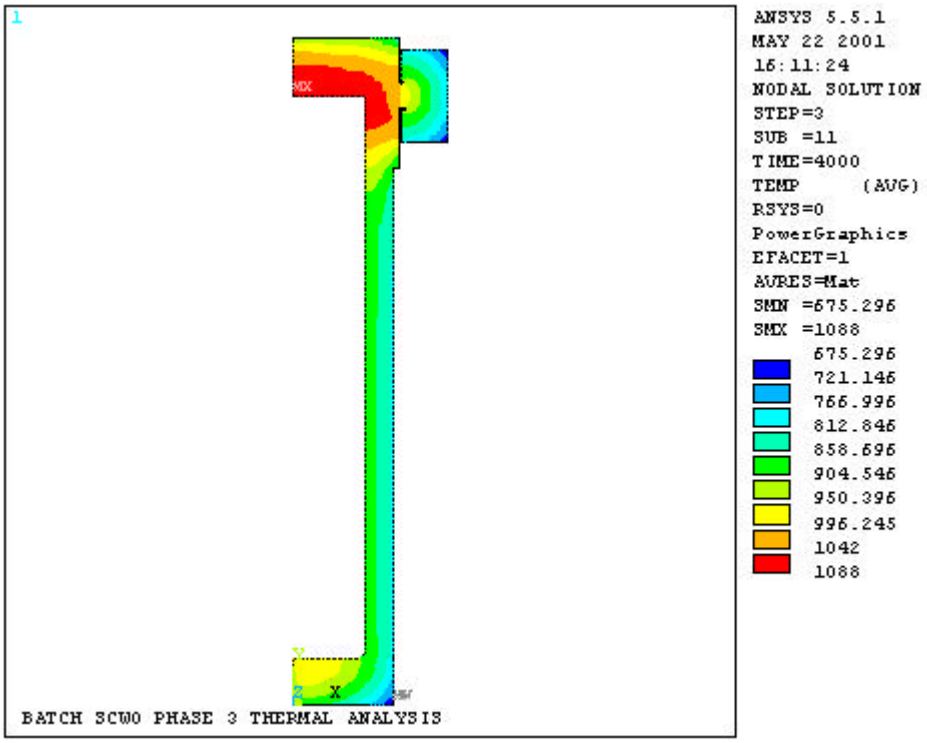
The temperature contour plots contained in this section are for selected time steps in the ANSYS solution for the large vessel cooldown transient. The forced convection film coefficient derived in Section 7.4 is applied uniformly to the outer surfaces of the model with a bulk air temperature of 70°F. The model is initially set to a uniform 1200°F. As can be seen in the plots the model is between 76°F and 128°F at 46800 sec.



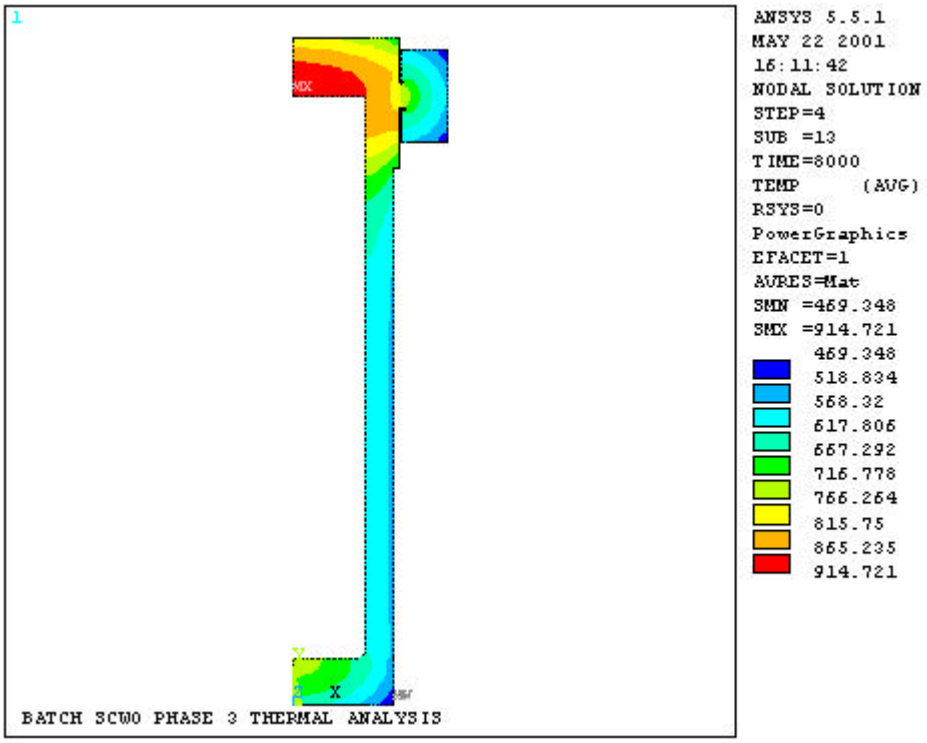
Batch SCWO Large Vessel 1000 sec



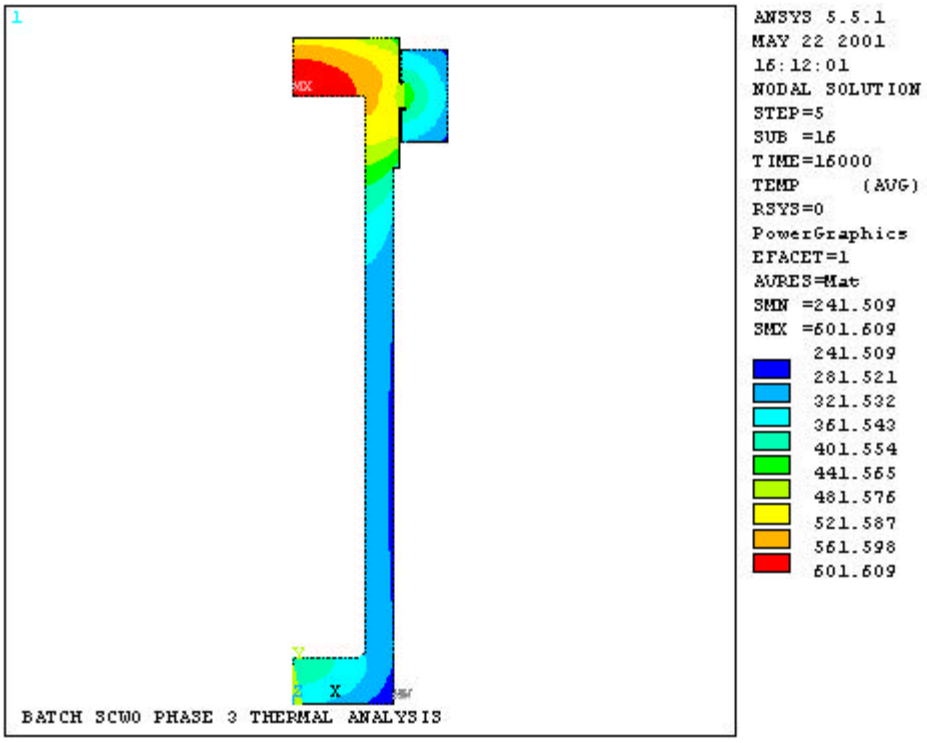
Batch SCWO Large Vessel 2000 sec



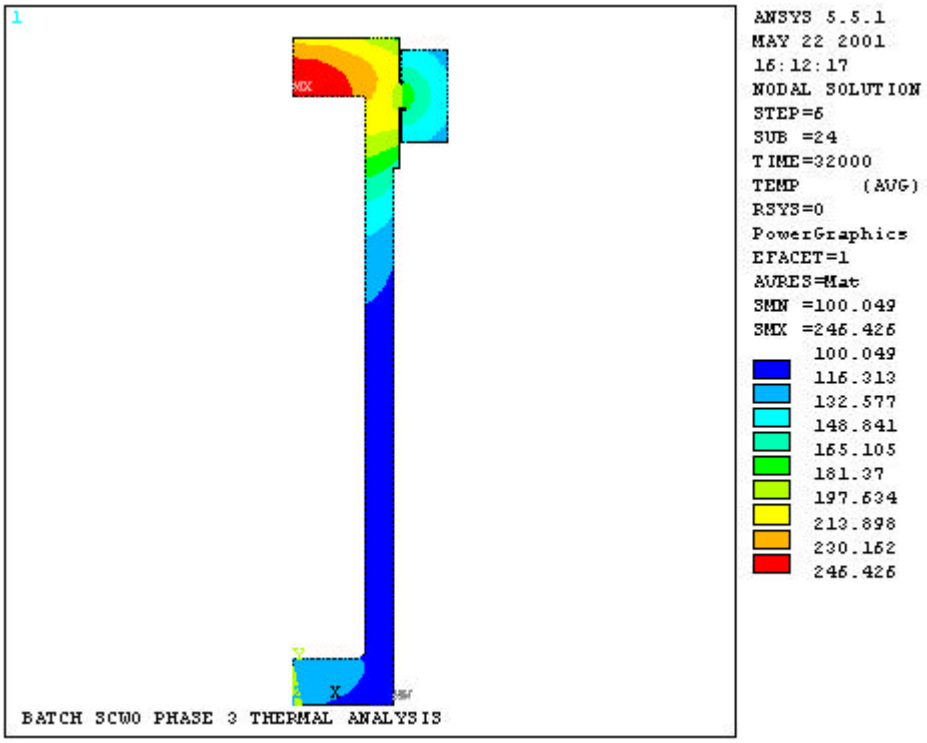
Batch SCWO Large Vessel 4000 sec



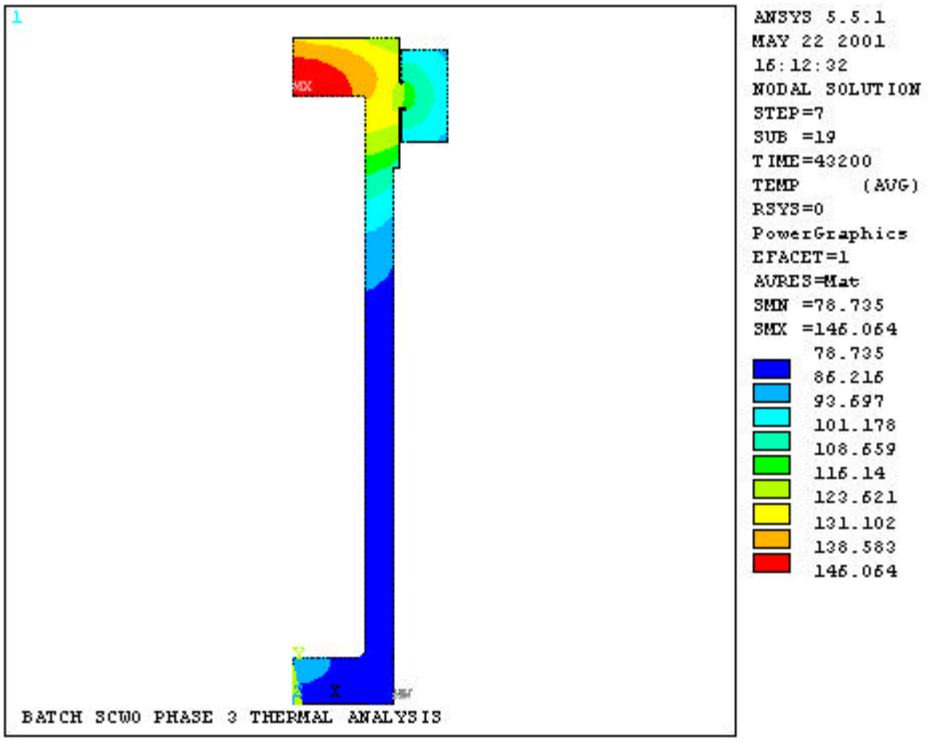
Batch SCWO Large Vessel 8000 sec



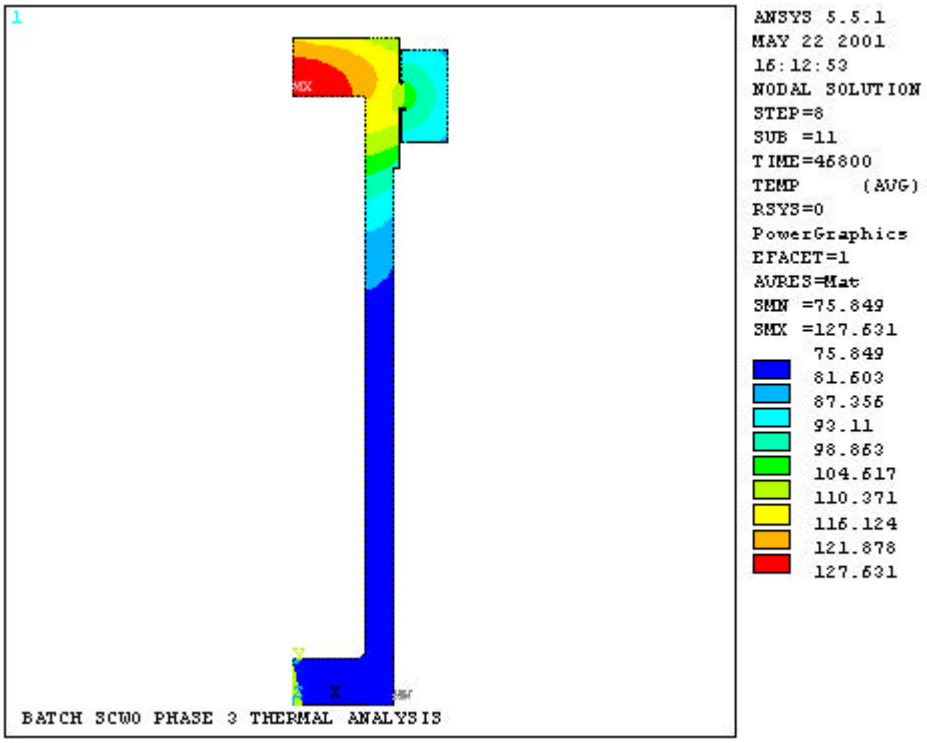
Batch SCWO Large Vessel 16,000 sec



Batch SCWO Large Vessel 32,000 sec



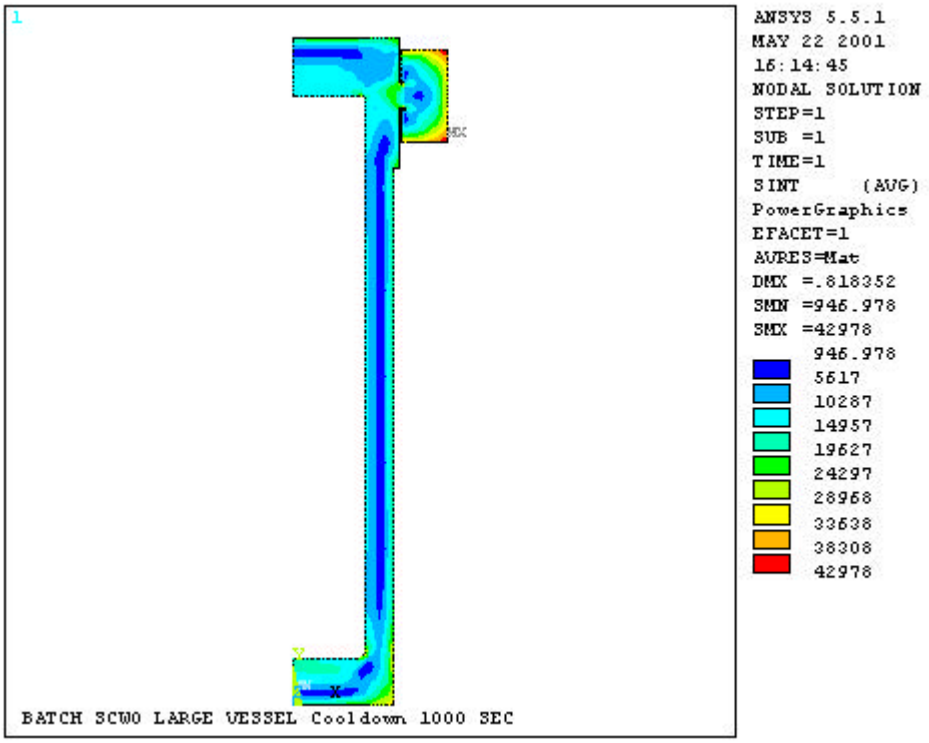
Batch SCWO Large Vessel 43,200 sec

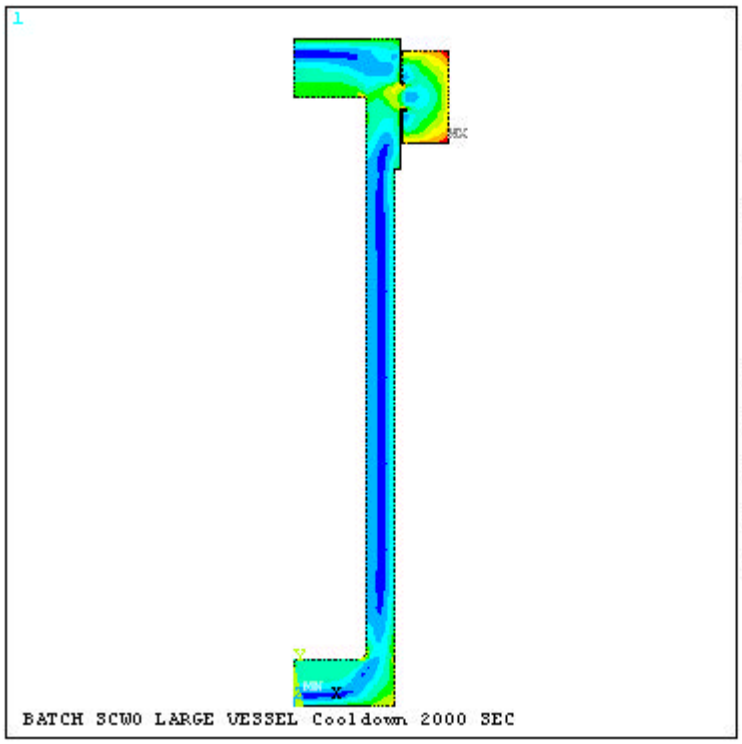


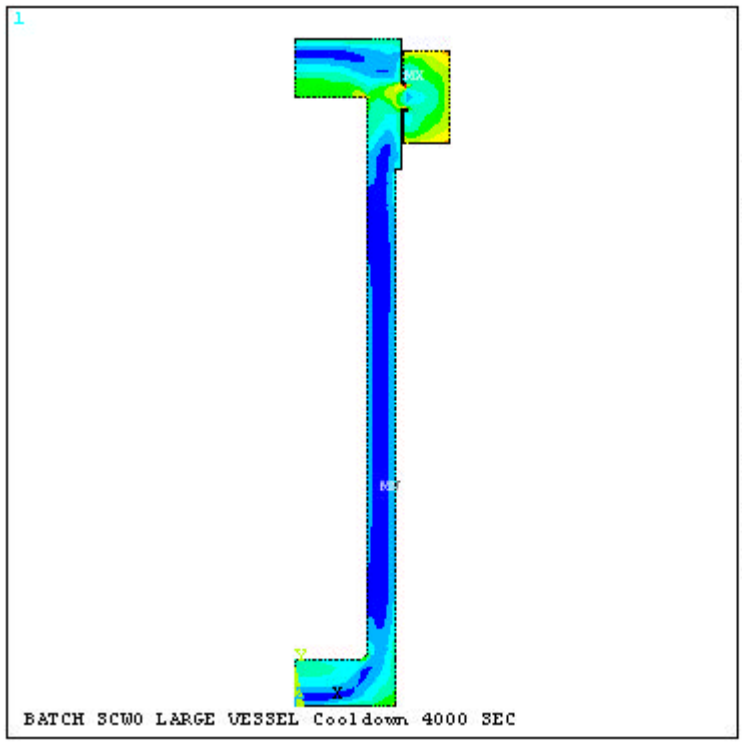
Batch SCWO Large Vessel 46,800 sec

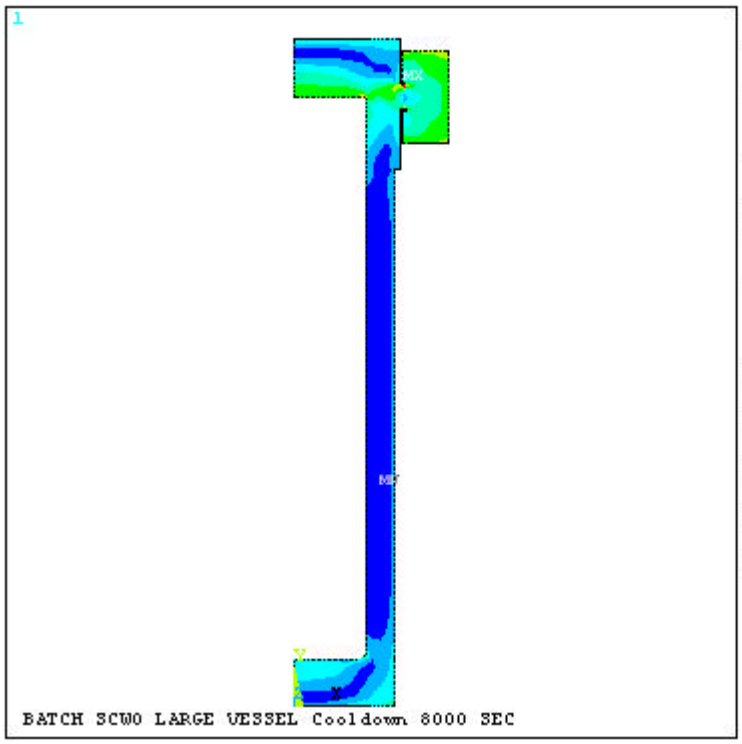
7.14 Large Vessel Stress Contour Plots – Cooldown Transient

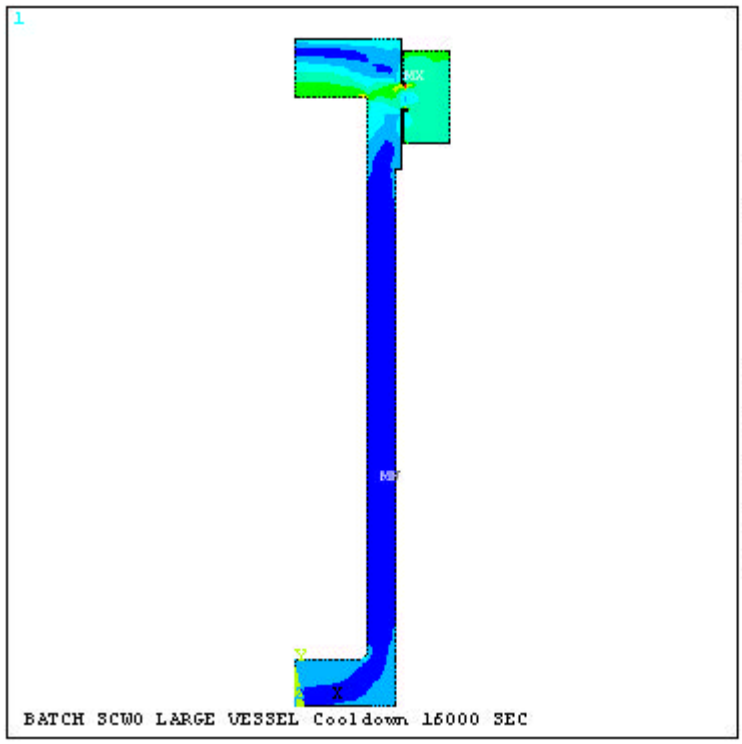
The stress intensity contour plots contained in this section are calculated for the temperature distribution corresponding to the selected time steps in the ANSYS solution for the large vessel cool down transient. The maximum stress intensity is located in the clamp/flange, occurs at 8000 sec. and is equal to 76587 psi. Note that results presented for the clamp are only for informational purposes as the model is only relevant for the shell and lower head.

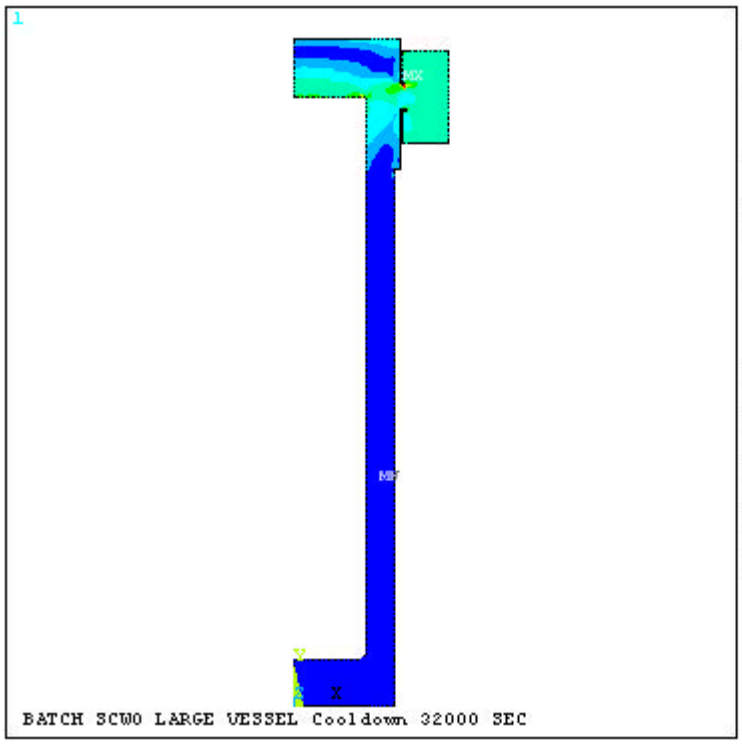


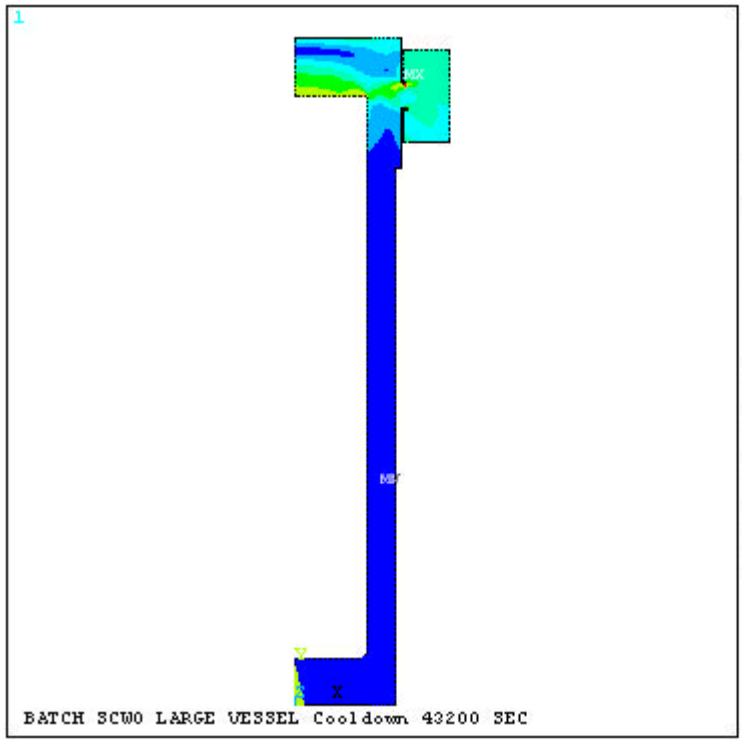

1
ANSYS 5.5.1
MAY 22 2001
15:15:06
NODAL SOLUTION
STEP=2
SUB =1
TIME=2
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.747882
SMN =460.421
SMX =47879
460.421
5729
10998
16267
21535
26804
32073
37341
42610
47879
BATCH SCWO LARGE VESSEL Cooldown 2000 SEC

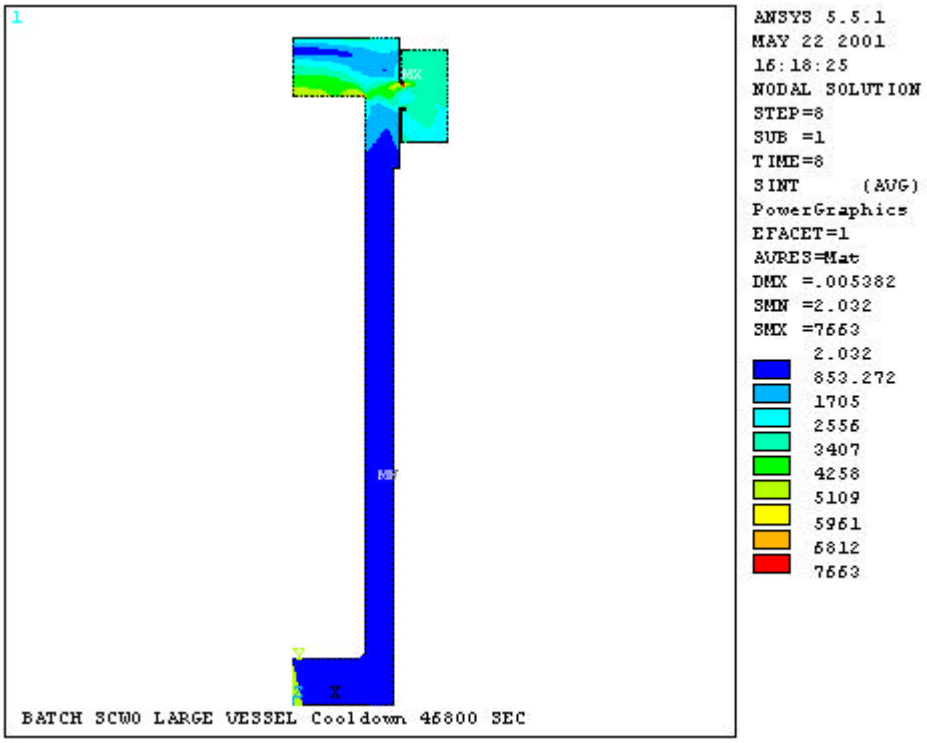

1
ANSYS 5.5.1
MAY 22 2001
15:15:25
NODAL SOLUTION
STEP=3
SUB =1
TIME=3
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.632392
SMN =1279
SMX =59672
1279
7767
14255
20744
27232
33720
40208
46696
53184
59672
BATCH SCWO LARGE VESSEL Cooldown 4000 SEC


1
MX
MN
BATCH SCW0 LARGE VESSEL Cooldown 8000 SEC
ANSYS 5.5.1
MAY 22 2001
15:15:47
NODAL SOLUTION
STEP=4
SUB =1
TIME=4
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.449116
SMN =1060
SMX =76587
1060
9452
17844
26236
34627
43019
51411
59803
68195
76587


1
MX
MN
BATCH SCW0 LARGE VESSEL Cooldown 16000 SEC
ANSYS 5.5.1
MAY 22 2001
15:17:16
NODAL SOLUTION
STEP=5
SUB =1
TIME=5
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.226749
SMN =461.559
SMX =65218
461.559
7657
14852
22047
29242
36437
43632
50827
58022
65218

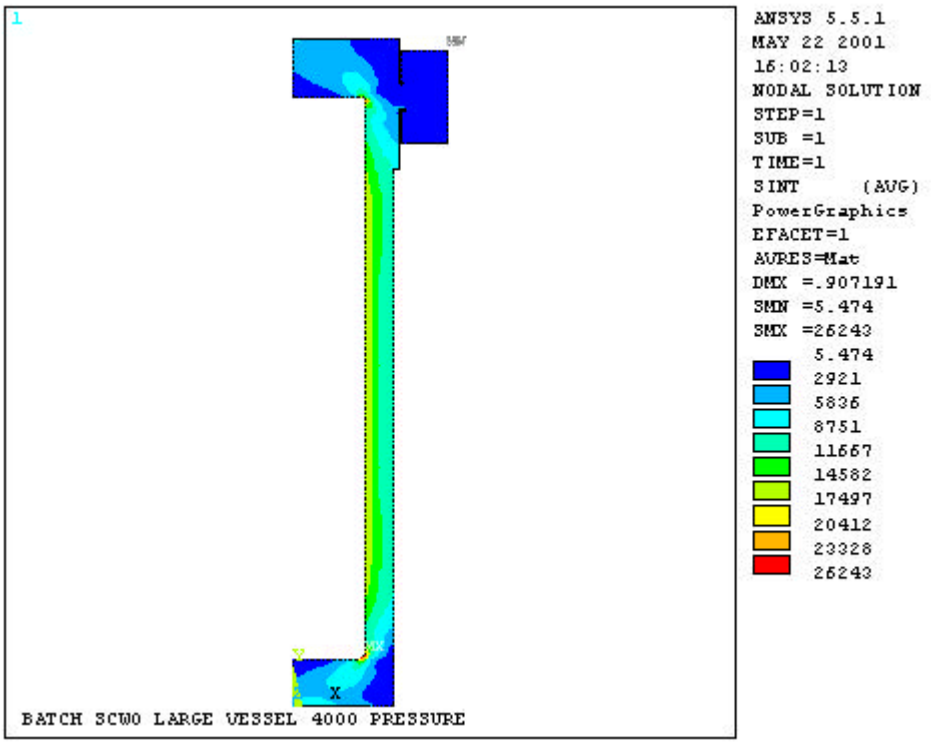

1
MX
MN
BATCH SCW0 LARGE VESSEL Cooldown 32000 SEC
ANSYS 5.5.1
MAY 22 2001
15:17:40
NODAL SOLUTION
STEP=6
SUB =1
TIME=6
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.045
SMN =63.575
SMX =40370
63.575
4542
9020
13499
17977
22456
26934
31413
35891
40370


1
MX
MN
BATCH SCW0 LARGE VESSEL Cooldown 43200 SEC
ANSYS 5.5.1
MAY 22 2001
15:18:02
NODAL SOLUTION
STEP=7
SUB =1
TIME=7
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.009334
SMN =10.628
SMX =11788
10.628
1319
2628
3937
5245
6554
7863
9171
10480
11788


1
MX
MN
BATCH SCW0 LARGE VESSEL Cooldown 46800 SEC
ANSYS 5.5.1
MAY 22 2001
16:18:25
NODAL SOLUTION
STEP=8
SUB =1
TIME=8
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.005382
SMN =2.032
SMX =7663
2.032
853.272
1705
2556
3407
4258
5109
5961
6812
7663

7.15 Large Vessel Stress Contour Plots – Pressure

A pressure load of 4000 psi is applied to the inner surfaces of the model and the resulting stress intensity contours are shown in the plot below. Maximum pressure stress occurs at the shell to bottom head fillet.



7.16 Power Input for Heatup

Small Vessel

Area: Heads: $\pi * (5.375in)^2 * 2 = 182\ in^2$
Wall: $\pi * 5.375in * 2 * 24in = 811\ in^2$

Power: Heads: $182\ in^2 * 11\ Watts/\ in^2 = 2{,}002\ Watts$
Wall: $811\ in^2 * 8\ Watts/\ in^2 = 6{,}488\ Watts$

Total = 8,490 Watts **Use 9 kW**

Large Vessel

Area: Heads: $\pi * (13.875in)^2 * 2 = 1210\ in^2$
Wall: $\pi * 13.875in * 2 * 78in = 6800\ in^2$

Power: Heads: $1210\ in^2 * 11\ Watts/\ in^2 = 13{,}310\ Watts$
Wall: $6800\ in^2 * 8\ Watts/\ in^2 = 54{,}400\ Watts$

Total = 67,710 Watts **Use 68 kW**

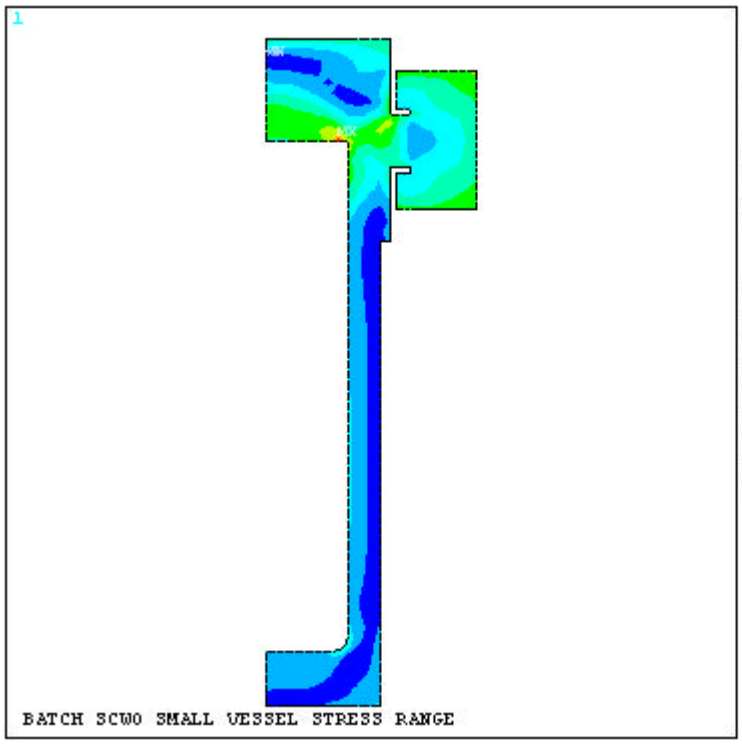
7.17 Fatigue Analysis

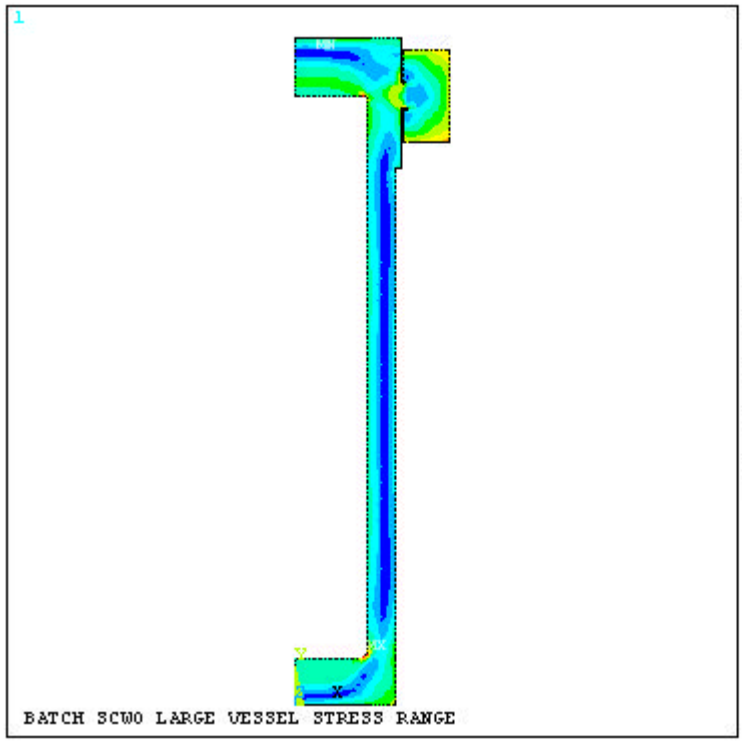
The ANSYS heatup, cooldown, and pressure stress results are post-processed to determine the maximum stress intensity range for each vessel. Only locations in the shell and lower head are considered since the closure/flange/clamp are not within the scope of this analysis. The maximum stress range occurs between the heatup plus pressure minus cooldown load cases and occurs in the vessel shell to lower head radii. The maximum stress intensity range and allowable cycles based on the design fatigue curve (Figure 4.3-1) are summarized below. ANSYS stress contour plots of the stress intensity range are shown.

Table 7.17-1 Fatigue Results

Vessel	Stress Intensity Range ksi	Allowable Cycles
Small	95*	1600
Large	110	110

* Note the maximum stress range is conservatively taken from the closure head region which envelopes the shell and lower head results.


1
ANSYS 5.5.1
MAY 24 2001
12:43:45
NODAL SOLUTION
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.083192
SMN =515.529
SMX =94154
515.529
10920
21324
31728
42133
52537
62941
73346
83750
94154
BATCH SCWO SMALL VESSEL STRESS RANGE


1
ANSYS 5.5.1
MAY 24 2001
12:48:16
NODAL SOLUTION
SINT (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.277122
SMN =977.28
SMX =107731
977.28
12839
24700
36562
48423
60285
72146
84008
95869
107731
BATCH SCWO LARGE VESSEL STRESS RANGE

7.18 Munition Detonation In Large Vessel

In addition to processing at SCWO conditions the large vessel is required to withstand the dynamic forces associated with detonation of both the munition burster charge and any shape charges used to access the munition. These detonations would occur with the vessel at room temperature. The Batch SCWO vessel is designed with the same internal diameter as the EDS Phase 1 vessel and has approximately twice the volume. Consequently, the Batch SCWO vessel could incorporate the same fragment suppression system which is provided for the EDS to absorb shock from high velocity fragments.

A fatigue/ life cycle analysis was performed on the EDS Vessel by Sandia National Laboratories and documented in a report dated August 15, 2000. Their conclusions were that for a 1.25 pound bare charge, the predicted peak pressure in the vessel is 19,000 psi with a maximum predicted stress of 21000 psi on the inner surface. Although the results are dependent on the specific vessel geometry, given that the Batch SCWO Vessel is a larger volume and almost twice the wall thickness of the EDS vessel, it is reasonable to expect that the maximum stresses due to the same detonation would not exceed 21000 psi in the Batch SCWO vessel wall. Room temperature strength of UNS N06617 is higher than EDS-1 material of construction (Allowable tensile of 23.3 ksi @100F vs. 13.0 ksi @ 1250F). A stress of this magnitude would be enveloped by the SCWO conditions and would not result in a reduction in the fatigue life. Note that the 1.25 pound explosive charge envelopes the explosive weight of the 4.2 inch mortar, the 75 mm artillery round, and the Livens projectile (Reference 7).

8. ANSYS INPUT LISTINGS

8.1 Small Vessel Thermal Analysis – Heatup Transient

```
/PREP7
/TITLE, BATCH SCWO PHASE 2 THERMAL
ANALYSIS FLAT HEAD
!*
ET,1,PLANE55
!*
KEYOPT,1,1,0
KEYOPT,1,3,1
KEYOPT,1,4,0
KEYOPT,1,8,0
KEYOPT,1,9,0
!*
MPTEMP,1,78,200,400,600,800,1000,
MPTEMP,7,1200, , , , , ,
MPDATA,KXX,1,1,1.813e-4,1.948e-
4,2.180e-4,2.411e-4,2.643e-
4,2.874e-4,
MPDATA,KXX,1,7,3.106e-4, , , , , ,
MPDATA,ALPX,1,1,0.0,6.4e-6,7.0e-
6,7.4e-6,7.6e-6,7.7e-6,
MPDATA,ALPX,1,7,8.0e-6, , , , , ,
MPDATA,C,1,1,.1,.104,.111,.117,.12
4,.131,
MPDATA,C,1,7,.137, , , , , ,
MPDATA,DENS,1,1,0.302,0.302,0.302,
0.302,0.302,0.302,
MPDATA,DENS,1,7,0.302, , , , , ,
MPDATA,EX,1,1,30.6e6,30.0e6,29.0e6
,28.0e6,26.9e6,25.8e6,
MPDATA,EX,1,7,24.6e6, , , , , ,
MPDATA,GXY,1,1,11.8e6,11.6e6,11.2e
6,10.8e6,10.4e6,9.9e6,
MPDATA,GXY,1,7,9.5e6, , , , , ,
MPDATA,PRXY,1,1,0.3,0.3,0.3,0.3,0.
3,0.3,
MPDATA,PRXY,1,7,0.3, , , , , ,
!*
K,1,0,2.25
K,2,3.875,2.25
K,3,5.375,2.25
K,4,,4.75,,
LSTR,       1,       2
LSTR,       2,       3
LSTR,       1,       4
FLST,2,2,4,ORDE,2
FITEM,2,1
FITEM,2,-2
ADRAG,P51X, , , , , ,       3
K,8,3.875,24,,
K,9,3.875,27.5,,
K,10,3.875,28.75,,
K,11,3.875,30.0
K,12,3.875,33.5
LSTR,       6,       8
LSTR,       8,       9
LSTR,       9,      10
LSTR,      10,      11
LSTR,      11,      12
FLST,8,5,4
FITEM,8,9
FITEM,8,10
FITEM,8,11
FITEM,8,12
FITEM,8,13
ADRAG,       7, , , , , ,P51X
K,23,0,28.75,,
LSTR,      10,      23
FLST,2,2,4,ORDE,2
FITEM,2,12
FITEM,2,-13
ADRAG,P51X, , , , , ,      29
K,27,5.875,24,,
LSTR,      14,      27
FLST,2,4,4,ORDE,4
FITEM,2,19
FITEM,2,22
FITEM,2,25
FITEM,2,28
ADRAG,P51X, , , , , ,      35
K,33,6.8125,28.75,,
LSTR,      30,      33
FLST,2,2,4,ORDE,2
FITEM,2,39
FITEM,2,41
ADRAG,P51X, , , , , ,      45
NUMMRG,KP,.1, ,
K,37,6.1875,28,,
K,37,6.1875,30.25,,
K,37,6.8125,30.25,,
K,38,6.8125,32,,
K,39,9.9,28.75,,
LSTR,      36,      37
```

```
LSTR,      37,      38
LSTR,      33,      39
FLST,2,3,4,ORDE,3
FITEM,2,5
FITEM,2,15
FITEM,2,49
ADRAG,P51X, , , , , ,      18
K,40,6.125,30.25,,
LSTR,      37,      40
ADRAG,      15, , , , , ,      52
K,41,6.8125,27.25,,
K,42,6.8125,25.5,,
LSTR,      34,      41
LSTR,      41,      42
FLST,8,3,4
FITEM,8,46
FITEM,8,56
FITEM,8,57
ADRAG,      18, , , , , ,P51X
K,46,6.125,25.5,,
LSTR,      42,      46
ADRAG,      57, , , , , ,      67
NUMMRG,KP,0.1, ,
FLST,2,3,5,ORDE,2
FITEM,2,1
FITEM,2,-3
ADELE,P51X
LPLOT
!*
LFILLT,4,9,0.75, ,
FLST,2,4,3
FITEM,2,34
FITEM,2,4
FITEM,2,1
FITEM,2,2
A,P51X
FLST,2,5,3
FITEM,2,39
FITEM,2,34
FITEM,2,2
FITEM,2,3
FITEM,2,7
A,P51X
FLST,2,4,3
FITEM,2,39
FITEM,2,7
FITEM,2,14
FITEM,2,8
A,P51X
NUMMRG,KP,0.1, ,
ESIZE,0.5,0,
AATT,       1, ,   1,       0
MSHKEY,0
FLST,5,23,5,ORDE,2
FITEM,5,1
FITEM,5,-23
CM,_Y,AREA
ASEL, , , ,P51X
CM,_Y1,AREA
CHKMSH,'AREA'
CMSEL,S,_Y
!*
AMESH,_Y1
!*
CMDEL,_Y
CMDEL,_Y1
CMDEL,_Y2
!*
ANTYPE,4
!*
TUNIF,70.
!*
FLST,2,3,4,ORDE,3
FITEM,2,26
FITEM,2,34
FITEM,2,44
/GO
!*
!*TOP HEAD
SFL,P51X,HFLUX,0.019,
SFL,P51X,HFLUX,0.019
!*
FLST,5,6,2,ORDE,4
FITEM,5,323
FITEM,5,-325
FITEM,5,340
FITEM,5,-342
CM,_Y,ELEM
ESEL, , , ,P51X
CM,_Y1,ELEM
CMSEL,S,_Y
CMDELE,_Y
!*
/GO
!*
!*TOP HEAD OD
SFE,_Y1,2,HFLUX, ,0.015, , ,
CMDELE,_Y1
!*
FLST,2,2,4,ORDE,2
FITEM,2,1
FITEM,2,-2
/GO
!*
!*BOTTOM HEAD
SFL,P51X,HFLUX,0.010,
SFL,P51X,HFLUX,0.010
!*
```

```
FLST,2,3,4,ORDE,3
FITEM,2,8
FITEM,2,16
FITEM,2,35
/GO
!*
!*WALL
SFL,P51X,HFLUX,0.007,
SFL,P51X,HFLUX,0.007
!*
FLST,2,10,4,ORDE,10
FITEM,2,21
FITEM,2,24
FITEM,2,31
FITEM,2,48
FITEM,2,55
FITEM,2,60
FITEM,2,63
FITEM,2,-64
FITEM,2,66
FITEM,2,-67
/GO
!*
!*CLAMP
SFL,P51X,HFLUX,0.009,
SFL,P51X,HFLUX,0.009
!*
TIME,300
AUTOTS,-1
DELTIM, ,1,300,1
KBC,1
TSRES,ERASE
LSWRITE,1,
!*
TIME,600
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,2,
!*
TIME,1000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,3,
!*
TIME,2000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,4,
!*
TIME,3000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,5,
!*
TIME,4000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,6,
!*
TIME,5000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,7,
!*
TIME,6000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,8,
!*
TIME,6500
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,9,
!*
SFLDELE,ALL,ALL
FLST,2,4,1,ORDE,4
FITEM,2,459
FITEM,2,-460
FITEM,2,476
FITEM,2,-477
SFDELE,P51X,HFLUX
TIME,7200
AUTOTS,-1
KBC,1
TSRES,ERASE
LSWRITE,10,
```

8.2 Small Vessel Stress Analysis – Heatup Transient

```
/PREP7
/TITLE, BATCH SCWO SMALL VESSEL
HEATUP STRESS
!*
ET,1,PLANE55
!*
KEYOPT,1,1,0
KEYOPT,1,3,1
KEYOPT,1,4,0
KEYOPT,1,8,0
KEYOPT,1,9,0
!*
MPTEMP,1,78,200,400,600,800,1000,
MPTEMP,7,1200, , , , , ,
MPDATA,KXX,1,1,1.813e-4,1.948e-
4,2.180e-4,2.411e-4,2.643e-
4,2.874e-4,
MPDATA,KXX,1,7,3.106e-4, , , , , ,
MPDATA,ALPX,1,1,0.0,6.4e-6,7.0e-
6,7.4e-6,7.6e-6,7.7e-6,
MPDATA,ALPX,1,7,8.0e-6, , , , , ,
MPDATA,C,1,1,.1,.104,.111,.117,.12
4,.131,
MPDATA,C,1,7,.137, , , , , ,
MPDATA,DENS,1,1,0.302,0.302,0.302,
0.302,0.302,0.302,
MPDATA,DENS,1,7,0.302, , , , , ,
MPDATA,EX,1,1,30.6e6,30.0e6,29.0e6
,28.0e6,26.9e6,25.8e6,
MPDATA,EX,1,7,24.6e6, , , , , ,
MPDATA,GXY,1,1,11.8e6,11.6e6,11.2e
6,10.8e6,10.4e6,9.9e6,
MPDATA,GXY,1,7,9.5e6, , , , , ,
MPDATA,PRXY,1,1,0.3,0.3,0.3,0.3,0.
3,0.3,
MPDATA,PRXY,1,7,0.3, , , , , ,
!*
K,1,0,2.25
K,2,3.875,2.25
K,3,5.375,2.25
K,4,,4.75,,
LSTR,       1,       2
LSTR,       2,       3
LSTR,       1,       4
FLST,2,2,4,ORDE,2
FITEM,2,1
FITEM,2,-2
ADRAG,P51X, , , , , ,       3
K,8,3.875,24,,
K,9,3.875,27.5,,
K,10,3.875,28.75,,
K,11,3.875,30.0
K,12,3.875,33.5
LSTR,       6,       8
LSTR,       8,       9
LSTR,       9,      10
LSTR,      10,      11
LSTR,      11,      12
FLST,8,5,4
FITEM,8,9
FITEM,8,10
FITEM,8,11
FITEM,8,12
FITEM,8,13
ADRAG,       7, , , , , ,P51X
K,23,0,28.75,,
LSTR,      10,      23
FLST,2,2,4,ORDE,2
FITEM,2,12
FITEM,2,-13
ADRAG,P51X, , , , , ,      29
K,27,5.875,24,,
LSTR,      14,      27
FLST,2,4,4,ORDE,4
FITEM,2,19
FITEM,2,22
FITEM,2,25
FITEM,2,28
ADRAG,P51X, , , , , ,      35
K,33,6.8125,28.75,,
LSTR,      30,      33
FLST,2,2,4,ORDE,2
FITEM,2,39
FITEM,2,41
ADRAG,P51X, , , , , ,      45
NUMMRG,KP,.1, ,
K,37,6.1875,28,,
K,37,6.1875,30.25,,
K,37,6.8125,30.25,,
K,38,6.8125,32,,
K,39,9.9,28.75,,
LSTR,      36,      37
```

```
LSTR,      37,      38
LSTR,      33,      39
FLST,2,3,4,ORDE,3
FITEM,2,5
FITEM,2,15
FITEM,2,49
ADRAG,P51X, , , , , ,      18
K,40,6.125,30.25,,
LSTR,      37,      40
ADRAG,      15, , , , , ,      52
K,41,6.8125,27.25,,
K,42,6.8125,25.5,,
LSTR,      34,      41
LSTR,      41,      42
FLST,8,3,4
FITEM,8,46
FITEM,8,56
FITEM,8,57
ADRAG,      18, , , , , ,P51X
K,46,6.125,25.5,,
LSTR,      42,      46
ADRAG,      57, , , , , ,      67
NUMMRG,KP,0.1, ,
FLST,2,3,5,ORDE,2
FITEM,2,1
FITEM,2,-3
ADELE,P51X
LPLOT
!*
LFILLT,4,9,0.75, ,
FLST,2,4,3
FITEM,2,34
FITEM,2,4
FITEM,2,1
FITEM,2,2
A,P51X
FLST,2,5,3
FITEM,2,39
FITEM,2,34
FITEM,2,2
FITEM,2,3
FITEM,2,7
A,P51X
FLST,2,4,3
FITEM,2,39
FITEM,2,7
FITEM,2,14
FITEM,2,8
A,P51X
NUMMRG,KP,0.1, ,
ESIZE,0.5,0,
AATT,       1, ,   1,       0
MSHKEY,0
FLST,5,23,5,ORDE,2
FITEM,5,1
FITEM,5,-23
CM,_Y,AREA
ASEL, , , ,P51X
CM,_Y1,AREA
CHKMSH,'AREA'
CMSEL,S,_Y
!*
AMESH,_Y1
!*
CMDEL,_Y
CMDEL,_Y1
CMDEL,_Y2
!*
ETCHG,TTS
!*
KEYOPT,1,1,0
KEYOPT,1,2,0
KEYOPT,1,3,1
KEYOPT,1,5,0
KEYOPT,1,6,0
!*
ANTYPE,0
FLST,2,1,1,ORDE,1
FITEM,2,9
!*
/GO
D,P51X, ,0.0, , , ,UY, , , , ,
!*
/TITLE, BATCH SCWO SMALL VESSEL
Heatup 300 SEC
LDREAD,TEMP,,,300,
,SmallHeatR,rth,
LSWRITE,1,
!*
/TITLE, BATCH SCWO SMALL VESSEL
Heatup 600 SEC
LDREAD,TEMP,,,600,
,SmallHeatR,rth,
LSWRITE,2,
!*
/TITLE, BATCH SCWO SMALL VESSEL
Heatup 1000 SEC
LDREAD,TEMP,,,1000,
,SmallHeatR,rth,
LSWRITE,3,
!*
/TITLE, BATCH SCWO SMALL VESSEL
Heatup 2000 SEC
LDREAD,TEMP,,,2000,
,SmallHeatR,rth,
LSWRITE,4,
!*
```

```
/TITLE, BATCH SCWO SMALL VESSEL
Heatup 3000 SEC
LDREAD,TEMP,,,3000,
,SmallHeatR,rth,
LSWRITE,5,
!*
/TITLE, BATCH SCWO SMALL VESSEL
Heatup 4000 SEC
LDREAD,TEMP,,,4000,
,SmallHeatR,rth,
LSWRITE,6,
!*
/TITLE, BATCH SCWO SMALL VESSEL
Heatup 5000 SEC
LDREAD,TEMP,,,5000,
,SmallHeatR,rth,
LSWRITE,7,
!*
```

```
/TITLE, BATCH SCWO SMALL VESSEL
Heatup 6000 SEC
LDREAD,TEMP,,,6000,
,SmallHeatR,rth,
LSWRITE,8,
!*
/TITLE, BATCH SCWO SMALL VESSEL
Heatup 6500 SEC
LDREAD,TEMP,,,6500,
,SmallHeatR,rth,
LSWRITE,9,
!*
/TITLE, BATCH SCWO SMALL VESSEL
Heatup 7200 SEC
LDREAD,TEMP,,,7200,
,SmallHeatR,rth,
LSWRITE,10,
!*
```

8.3 Small Vessel Thermal Analysis – Cooldown Transient

```
/PREP7
/TITLE, BATCH SCWO PHASE 2 THERMAL
ANALYSIS FLAT HEAD
!*
ET,1,PLANE55
!*
KEYOPT,1,1,0
KEYOPT,1,3,1
KEYOPT,1,4,0
KEYOPT,1,8,0
KEYOPT,1,9,0
!*
MPTEMP,1,78,200,400,600,800,1000,
MPTEMP,7,1200, , , , , ,
MPDATA,KXX,1,1,1.813e-4,1.948e-
4,2.180e-4,2.411e-4,2.643e-
4,2.874e-4,
MPDATA,KXX,1,7,3.106e-4, , , , , ,
MPDATA,ALPX,1,1,0.0,6.4e-6,7.0e-
6,7.4e-6,7.6e-6,7.7e-6,
MPDATA,ALPX,1,7,8.0e-6, , , , , ,
MPDATA,C,1,1,.1,.104,.111,.117,.12
4,.131,
MPDATA,C,1,7,.137, , , , , ,
MPDATA,DENS,1,1,0.302,0.302,0.302,
0.302,0.302,0.302,
MPDATA,DENS,1,7,0.302, , , , , ,
MPDATA,EX,1,1,30.6e6,30.0e6,29.0e6
,28.0e6,26.9e6,25.8e6,
MPDATA,EX,1,7,24.6e6, , , , , ,
MPDATA,GXY,1,1,11.8e6,11.6e6,11.2e
6,10.8e6,10.4e6,9.9e6,
MPDATA,GXY,1,7,9.5e6, , , , , ,
MPDATA,PRXY,1,1,0.3,0.3,0.3,0.3,0.
3,0.3,
MPDATA,PRXY,1,7,0.3, , , , , ,
!*
K,1,0,2.25
K,2,3.875,2.25
K,3,5.375,2.25
K,4,,4.75,,
LSTR,       1,       2
LSTR,       2,       3
LSTR,       1,       4
FLST,2,2,4,ORDE,2
FITEM,2,1
FITEM,2,-2
ADRAG,P51X, , , , , ,       3
K,8,3.875,24,,
K,9,3.875,27.5,,
K,10,3.875,28.75,,
K,11,3.875,30.0
K,12,3.875,33.5
LSTR,       6,       8
LSTR,       8,       9
```

```
LSTR,       9,      10
LSTR,      10,      11
LSTR,      11,      12
FLST,8,5,4
FITEM,8,9
FITEM,8,10
FITEM,8,11
FITEM,8,12
FITEM,8,13
ADRAG,       7, , , , , ,P51X
K,23,0,28.75,,
LSTR,      10,      23
FLST,2,2,4,ORDE,2
FITEM,2,12
FITEM,2,-13
ADRAG,P51X, , , , , ,      29
K,27,5.875,24,,
LSTR,      14,      27
FLST,2,4,4,ORDE,4
FITEM,2,19
FITEM,2,22
FITEM,2,25
FITEM,2,28
ADRAG,P51X, , , , , ,      35
K,33,6.8125,28.75,,
LSTR,      30,      33
FLST,2,2,4,ORDE,2
FITEM,2,39
FITEM,2,41
ADRAG,P51X, , , , , ,      45
NUMMRG,KP,.1, ,
K,37,6.1875,28,,
K,37,6.1875,30.25,,
K,37,6.8125,30.25,,
K,38,6.8125,32,,
K,39,9.9,28.75,,
LSTR,      36,      37
LSTR,      37,      38
LSTR,      33,      39
FLST,2,3,4,ORDE,3
FITEM,2,5
FITEM,2,15
FITEM,2,49
ADRAG,P51X, , , , , ,      18
K,40,6.125,30.25,,
LSTR,      37,      40
ADRAG,      15, , , , , ,      52
K,41,6.8125,27.25,,
K,42,6.8125,25.5,,
LSTR,      34,      41
LSTR,      41,      42
FLST,8,3,4
FITEM,8,46
FITEM,8,56
FITEM,8,57
ADRAG,      18, , , , , ,P51X
K,46,6.125,25.5,,
LSTR,      42,      46
ADRAG,      57, , , , , ,      67
NUMMRG,KP,0.1, ,
FLST,2,3,5,ORDE,2
FITEM,2,1
FITEM,2,-3
ADELE,P51X
LPLOT
!*
LFILLT,4,9,0.75, ,
FLST,2,4,3
FITEM,2,34
FITEM,2,4
FITEM,2,1
FITEM,2,2
A,P51X
FLST,2,5,3
FITEM,2,39
FITEM,2,34
FITEM,2,2
FITEM,2,3
FITEM,2,7
A,P51X
FLST,2,4,3
FITEM,2,39
FITEM,2,7
FITEM,2,14
FITEM,2,8
A,P51X
NUMMRG,KP,0.1, ,
ESIZE,0.5,0,
AATT,       1, ,   1,       0
MSHKEY,0
FLST,5,23,5,ORDE,2
FITEM,5,1
FITEM,5,-23
CM,_Y,AREA
ASEL, , , ,P51X
CM,_Y1,AREA
CHKMSH,'AREA'
CMSEL,S,_Y
!*
AMESH,_Y1
!*
CMDEL,_Y
CMDEL,_Y1
CMDEL,_Y2
!*
ANTYPE,4
!*
TUNIF,1200.
```

```
FLST,2,18,4,ORDE,18
FITEM,2,1
FITEM,2,-2
FITEM,2,8
FITEM,2,16
FITEM,2,21
FITEM,2,24
FITEM,2,26
FITEM,2,31
FITEM,2,34
FITEM,2,-35
FITEM,2,44
FITEM,2,48
FITEM,2,55
FITEM,2,60
FITEM,2,63
FITEM,2,-64
FITEM,2,66
FITEM,2,-67
/GO
!*
SFL,P51X,CONV,1.35e-5, ,70.0,
FLST,5,6,2,ORDE,4
FITEM,5,323
FITEM,5,-325
FITEM,5,340
FITEM,5,-342
CM,_Y,ELEM
ESEL, , , ,P51X
CM,_Y1,ELEM
CMSEL,S,_Y
CMDELE,_Y
!*
/GO
!*
SFE,_Y1,2,CONV, ,1.35e-005
SFE,_Y1,2,CONV,2,70

CMDELE,_Y1
TIME,1000
AUTOTS,-1
DELTIM, ,1,1000,1
KBC,1
TSRES,ERASE
LSWRITE,1,
!*
TIME,2000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,2,
!*
TIME,4000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,3,
!*
TIME,8000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,4,
!*
TIME,12000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,5,
!*
TIME,16000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,6,
!*
TIME,18000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,7,
!*
```

8.4 Small Vessel Stress Analysis – Cooldown Transient

```
PREP7
/TITLE, BATCH SCWO SMALL VESSEL
COOLDOWN STRESS
!*
ET,1,PLANE55
!*
KEYOPT,1,1,0
KEYOPT,1,3,1
```

```
KEYOPT,1,4,0
KEYOPT,1,8,0
KEYOPT,1,9,0
!*
MPTEMP,1,78,200,400,600,800,1000,
MPTEMP,7,1200, , , , , ,
MPDATA,KXX,1,1,1.813e-4,1.948e-
4,2.180e-4,2.411e-4,2.643e-
4,2.874e-4,
MPDATA,KXX,1,7,3.106e-4, , , , , ,
MPDATA,ALPX,1,1,0.0,6.4e-6,7.0e-
6,7.4e-6,7.6e-6,7.7e-6,
MPDATA,ALPX,1,7,8.0e-6, , , , , ,
MPDATA,C,1,1,.1,.104,.111,.117,.12
4,.131,
MPDATA,C,1,7,.137, , , , , ,
MPDATA,DENS,1,1,0.302,0.302,0.302,
0.302,0.302,0.302,
MPDATA,DENS,1,7,0.302, , , , , ,
MPDATA,EX,1,1,30.6e6,30.0e6,29.0e6
,28.0e6,26.9e6,25.8e6,
MPDATA,EX,1,7,24.6e6, , , , , ,
MPDATA,GXY,1,1,11.8e6,11.6e6,11.2e
6,10.8e6,10.4e6,9.9e6,
MPDATA,GXY,1,7,9.5e6, , , , , ,
MPDATA,PRXY,1,1,0.3,0.3,0.3,0.3,0.
3,0.3,
MPDATA,PRXY,1,7,0.3, , , , , ,
!*
K,1,0,2.25
K,2,3.875,2.25
K,3,5.375,2.25
K,4,,4.75,,
LSTR,       1,       2
LSTR,       2,       3
LSTR,       1,       4
FLST,2,2,4,ORDE,2
FITEM,2,1
FITEM,2,-2
ADRAG,P51X, , , , , ,       3
K,8,3.875,24,,
K,9,3.875,27.5,,
K,10,3.875,28.75,,
K,11,3.875,30.0
K,12,3.875,33.5
LSTR,       6,       8
LSTR,       8,       9
LSTR,       9,      10
LSTR,      10,      11
LSTR,      11,      12
FLST,8,5,4
FITEM,8,9
FITEM,8,10
FITEM,8,11
FITEM,8,12
FITEM,8,13
ADRAG,       7, , , , , ,P51X
K,23,0,28.75,,
LSTR,      10,      23
FLST,2,2,4,ORDE,2
FITEM,2,12
FITEM,2,-13
ADRAG,P51X, , , , , ,      29
K,27,5.875,24,,
LSTR,      14,      27
FLST,2,4,4,ORDE,4
FITEM,2,19
FITEM,2,22
FITEM,2,25
FITEM,2,28
ADRAG,P51X, , , , , ,      35
K,33,6.8125,28.75,,
LSTR,      30,      33
FLST,2,2,4,ORDE,2
FITEM,2,39
FITEM,2,41
ADRAG,P51X, , , , , ,      45
NUMMRG,KP,.1, ,
K,37,6.1875,28,,
K,37,6.1875,30.25,,
K,37,6.8125,30.25,,
K,38,6.8125,32,,
K,39,9.9,28.75,,
LSTR,      36,      37
LSTR,      37,      38
LSTR,      33,      39
FLST,2,3,4,ORDE,3
FITEM,2,5
FITEM,2,15
FITEM,2,49
ADRAG,P51X, , , , , ,      18
K,40,6.125,30.25,,
LSTR,      37,      40
ADRAG,      15, , , , , ,      52
K,41,6.8125,27.25,,
K,42,6.8125,25.5,,
LSTR,      34,      41
LSTR,      41,      42
FLST,8,3,4
FITEM,8,46
FITEM,8,56
FITEM,8,57
ADRAG,      18, , , , , ,P51X
K,46,6.125,25.5,,
LSTR,      42,      46
ADRAG,      57, , , , , ,      67
NUMMRG,KP,0.1, ,
FLST,2,3,5,ORDE,2
```

```
FITEM,2,1
FITEM,2,-3
ADELE,P51X
LPLOT
!*
LFILLT,4,9,0.75, ,
FLST,2,4,3
FITEM,2,34
FITEM,2,4
FITEM,2,1
FITEM,2,2
A,P51X
FLST,2,5,3
FITEM,2,39
FITEM,2,34
FITEM,2,2
FITEM,2,3
FITEM,2,7
A,P51X
FLST,2,4,3
FITEM,2,39
FITEM,2,7
FITEM,2,14
FITEM,2,8
A,P51X
NUMMRG,KP,0.1, ,
ESIZE,0.5,0,
AATT,       1, ,   1,       0
MSHKEY,0
FLST,5,23,5,ORDE,2
FITEM,5,1
FITEM,5,-23
CM,_Y,AREA
ASEL, , , ,P51X
CM,_Y1,AREA
CHKMSH,'AREA'
CMSEL,S,_Y
!*
AMESH,_Y1
!*
CMDEL,_Y
CMDEL,_Y1
CMDEL,_Y2
!*
ETCHG,TTS
!*
KEYOPT,1,1,0
KEYOPT,1,2,0
KEYOPT,1,3,1
KEYOPT,1,5,0

!*
KEYOPT,1,6,0
!*
ANTYPE,0
FLST,2,1,1,ORDE,1
FITEM,2,9
!*
/GO
D,P51X, ,0.0, , , ,UY, , , , ,
!*
/TITLE, BATCH SCWO SMALL VESSEL
Cooldown 1000 SEC
LDREAD,TEMP,,,1000,
,SmallCoolR,rth,
LSWRITE,1,
!*
/TITLE, BATCH SCWO SMALL VESSEL
Cooldown 2000 SEC
LDREAD,TEMP,,,2000,
,SmallCoolR,rth,
LSWRITE,2,
!*
/TITLE, BATCH SCWO SMALL VESSEL
Cooldown 4000 SEC
LDREAD,TEMP,,,4000,
,SmallCoolR,rth,
LSWRITE,3,
!*
/TITLE, BATCH SCWO SMALL VESSEL
Cooldown 8000 SEC
LDREAD,TEMP,,,8000,
,SmallCoolR,rth,
LSWRITE,4,
!*
/TITLE, BATCH SCWO SMALL VESSEL
Cooldown 12000 SEC
LDREAD,TEMP,,,12000,
,SmallCoolR,rth,
LSWRITE,5,
!*
/TITLE, BATCH SCWO SMALL VESSEL
Cooldown 16000 SEC
LDREAD,TEMP,,,16000,
,SmallCoolR,rth,
LSWRITE,6,
!*
/TITLE, BATCH SCWO SMALL VESSEL
Cooldown 18000 SEC
LDREAD,TEMP,,,18000,
,SmallCoolR,rth,
LSWRITE,7,
```

8.5 Small Vessel Stress Analysis – Pressure

```
/PREP7
/TITLE, BATCH SCWO SMALL VESSEL
PRESSURE
!*
ET,1,PLANE55
!*
KEYOPT,1,1,0
KEYOPT,1,3,1
KEYOPT,1,4,0
KEYOPT,1,8,0
KEYOPT,1,9,0
!*
MPTEMP,1,78,200,400,600,800,1000,
MPTEMP,7,1200, , , , , ,
MPDATA,KXX,1,1,1.813e-4,1.948e-
4,2.180e-4,2.411e-4,2.643e-
4,2.874e-4,
MPDATA,KXX,1,7,3.106e-4, , , , , ,
MPDATA,ALPX,1,1,0.0,6.4e-6,7.0e-
6,7.4e-6,7.6e-6,7.7e-6,
MPDATA,ALPX,1,7,8.0e-6, , , , , ,
MPDATA,C,1,1,.1,.104,.111,.117,.12
4,.131,
MPDATA,C,1,7,.137, , , , , ,
MPDATA,DENS,1,1,0.302,0.302,0.302,
0.302,0.302,0.302,
MPDATA,DENS,1,7,0.302, , , , , ,
MPDATA,EX,1,1,30.6e6,30.0e6,29.0e6
,28.0e6,26.9e6,25.8e6,
MPDATA,EX,1,7,24.6e6, , , , , ,
MPDATA,GXY,1,1,11.8e6,11.6e6,11.2e
6,10.8e6,10.4e6,9.9e6,
MPDATA,GXY,1,7,9.5e6, , , , , ,
MPDATA,PRXY,1,1,0.3,0.3,0.3,0.3,0.
3,0.3,
MPDATA,PRXY,1,7,0.3, , , , , ,
!*
K,1,0,2.25
K,2,3.875,2.25
K,3,5.375,2.25
K,4,,4.75,,
LSTR,       1,       2
LSTR,       2,       3
LSTR,       1,       4
FLST,2,2,4,ORDE,2
FITEM,2,1
FITEM,2,-2
ADRAG,P51X, , , , , ,       3
K,8,3.875,24,,
K,9,3.875,27.5,,
K,10,3.875,28.75,,
K,11,3.875,30.0
K,12,3.875,33.5
LSTR,       6,       8
LSTR,       8,       9
LSTR,       9,      10
LSTR,      10,      11
LSTR,      11,      12
FLST,8,5,4
FITEM,8,9
FITEM,8,10
FITEM,8,11
FITEM,8,12
FITEM,8,13
ADRAG,       7, , , , , ,P51X
K,23,0,28.75,,
LSTR,      10,      23
FLST,2,2,4,ORDE,2
FITEM,2,12
FITEM,2,-13
ADRAG,P51X, , , , , ,      29
K,27,5.875,24,,
LSTR,      14,      27
FLST,2,4,4,ORDE,4
FITEM,2,19
FITEM,2,22
FITEM,2,25
FITEM,2,28
ADRAG,P51X, , , , , ,      35
K,33,6.8125,28.75,,
LSTR,      30,      33
FLST,2,2,4,ORDE,2
FITEM,2,39
FITEM,2,41
```

```
ADRAG,P51X, , , , , ,      45
NUMMRG,KP,.1, ,
K,37,6.1875,28,,
K,37,6.1875,30.25,,
K,37,6.8125,30.25,,
K,38,6.8125,32,,
K,39,9.9,28.75,,
LSTR,      36,      37
LSTR,      37,      38
LSTR,      33,      39
FLST,2,3,4,ORDE,3
FITEM,2,5
FITEM,2,15
FITEM,2,49
ADRAG,P51X, , , , , ,      18
K,40,6.125,30.25,,
LSTR,      37,      40
ADRAG,      15, , , , , ,      52
K,41,6.8125,27.25,,
K,42,6.8125,25.5,,
LSTR,      34,      41
LSTR,      41,      42
FLST,8,3,4
FITEM,8,46
FITEM,8,56
FITEM,8,57
ADRAG,      18, , , , , ,P51X
K,46,6.125,25.5,,
LSTR,      42,      46
ADRAG,      57, , , , , ,      67
NUMMRG,KP,0.1, ,
FLST,2,3,5,ORDE,2
FITEM,2,1
FITEM,2,-3
ADELE,P51X
LPLOT
!*
LFILLT,4,9,0.75, ,
FLST,2,4,3
FITEM,2,34
FITEM,2,4
FITEM,2,1
FITEM,2,2
A,P51X
FLST,2,5,3
FITEM,2,39
FITEM,2,34
FITEM,2,2
FITEM,2,29
FITEM,2,51
/GO
!*
SFL,P51X,PRES,4000,
LSWRITE,1,
FITEM,2,3
FITEM,2,7
A,P51X
FLST,2,4,3
FITEM,2,39
FITEM,2,7
FITEM,2,14
FITEM,2,8
A,P51X
NUMMRG,KP,0.1, ,
ESIZE,0.5,0,
AATT,       1, ,   1,       0
MSHKEY,0
FLST,5,23,5,ORDE,2
FITEM,5,1
FITEM,5,-23
CM,_Y,AREA
ASEL, , , ,P51X
CM,_Y1,AREA
CHKMSH,'AREA'
CMSEL,S,_Y
!*
AMESH,_Y1
!*
CMDEL,_Y
CMDEL,_Y1
CMDEL,_Y2
!*
ETCHG,TTS
!*
KEYOPT,1,1,0
KEYOPT,1,2,0
KEYOPT,1,3,1
KEYOPT,1,5,0
KEYOPT,1,6,0
!*
ANTYPE,0
FLST,2,1,1,ORDE,1
FITEM,2,9
!*
/GO
D,P51X, ,0.0, , , ,UY, , , , ,
!*
FLST,2,6,4,ORDE,5
FITEM,2,4
FITEM,2,9
FITEM,2,-11
```

8.6 Large Vessel Thermal Analysis – Heatup Transient

```
/PREP7
/TITLE, BATCH SCWO PHASE 3 THERMAL
ANALYSIS
!*
ET,1,PLANE55
!*
KEYOPT,1,1,0
KEYOPT,1,3,1
KEYOPT,1,4,0
KEYOPT,1,8,0
KEYOPT,1,9,0
!*
MPTEMP,1,78,200,400,600,800,1000,
MPTEMP,7,1200, , , , , ,
MPDATA,KXX,1,1,1.813e-4,1.948e-
4,2.180e-4,2.411e-4,2.643e-
4,2.874e-4,
MPDATA,KXX,1,7,3.106e-4, , , , , ,
MPDATA,ALPX,1,1,0.0,6.4e-6,7.0e-
6,7.4e-6,7.6e-6,7.7e-6,
MPDATA,ALPX,1,7,8.0e-6, , , , , ,
MPDATA,C,1,1,.1,.104,.111,.117,.12
4,.131,
MPDATA,C,1,7,.137, , , , , ,
MPDATA,DENS,1,1,0.302,0.302,0.302,
0.302,0.302,0.302,
MPDATA,DENS,1,7,0.302, , , , , ,
MPDATA,EX,1,1,30.6e6,30.0e6,29.0e6
,28.0e6,26.9e6,25.8e6,
MPDATA,EX,1,7,24.6e6, , , , , ,
MPDATA,GXY,1,1,11.8e6,11.6e6,11.2e
6,10.8e6,10.4e6,9.9e6,
MPDATA,GXY,1,7,9.5e6, , , , , ,
MPDATA,PRXY,1,1,0.3,0.3,0.3,0.3,0.
3,0.3,
MPDATA,PRXY,1,7,0.3, , , , , ,
!*
K,1,0,0
K,2,10.0
K,3,13.875
K,4,,6.375,,
LSTR,       1,       2
LSTR,       2,       3
LSTR,       1,       4
FLST,2,2,4,ORDE,2
FITEM,2,1
FITEM,2,-2
ADRAG,P51X, , , , , ,       3
K,8,10.0,74.375,,
K,9,10.0,82.75,,
K,10,10.0,84.375,,
K,11,10.0,86.0
K,12,10.0,92.375
LSTR,       6,       8
LSTR,       8,       9
LSTR,       9,      10
LSTR,      10,      11
LSTR,      11,      12
FLST,8,5,4
FITEM,8,9
FITEM,8,10
FITEM,8,11
FITEM,8,12
FITEM,8,13
ADRAG,       7, , , , ,P51X
K,23,0,84.375
LSTR,      10,      23
FLST,2,2,4,ORDE,2
FITEM,2,12
FITEM,2,-13
ADRAG,P51X, , , , , ,      29
K,27,14.625,74.375,,
LSTR,      14,      27
FLST,2,4,4,ORDE,4
FITEM,2,19
FITEM,2,22
FITEM,2,25
FITEM,2,28
ADRAG,P51X, , , , , ,      35
K,33,15.625,84.375,,
LSTR,      30,      33
FLST,2,2,4,ORDE,2
```

```
FITEM,2,39
FITEM,2,41
ADRAG,P51X, , , , , ,      45
NUMMRG,KP,.1, ,
K,37,15.625,86.25,,
K,38,15.625,90.71875,,
K,39,21.25,84.375,,
LSTR,      36,      37
LSTR,      37,      38
LSTR,      33,      39
FLST,2,3,4,ORDE,3
FITEM,2,5
FITEM,2,15
FITEM,2,49
ADRAG,P51X, , , , , ,      18
K,40,14.9685,86.25,,
LSTR,      37,      40
ADRAG,      15, , , , , ,      52
K,41,15.625,82.5,,
K,42,15.625,78.03125,,
LSTR,      34,      41
LSTR,      41,      42
FLST,8,3,4
FITEM,8,46
FITEM,8,56
FITEM,8,57
ADRAG,      18, , , , , ,P51X
K,46,14.9685,78.03125,,
LSTR,      42,      46
ADRAG,      57, , , , , ,      67
NUMMRG,KP,0.1, ,
FLST,2,3,5,ORDE,2
FITEM,2,1
FITEM,2,-3
ADELE,P51X
LPLOT
!*
LFILLT,9,4,1.0, ,
FLST,2,4,3
FITEM,2,39
FITEM,2,4
FITEM,2,1
FITEM,2,2
A,P51X
FLST,2,5,3
FITEM,2,34
FITEM,2,39
FITEM,2,2
FITEM,2,3
FITEM,2,7
A,P51X
FLST,2,4,3
FITEM,2,8
FITEM,2,34
FITEM,2,7
FITEM,2,14
A,P51X
APLOT
NUMMRG,KP,0.2, ,
AATT,       1, ,   1,       0
ESIZE,0.75,0,
MSHKEY,0
FLST,5,23,5,ORDE,2
FITEM,5,1
FITEM,5,-23
CM,_Y,AREA
ASEL, , , ,P51X
CM,_Y1,AREA
CHKMSH,'AREA'
CMSEL,S,_Y
!*
AMESH,_Y1
!*
CMDEL,_Y
CMDEL,_Y1
CMDEL,_Y2
ANTYPE,4
!*
TUNIF,70.
FLST,2,3,4,ORDE,3
FITEM,2,26
FITEM,2,34
FITEM,2,44
/GO
!*
!*TOP HEAD
SFL,P51X,HFLUX,0.014,
SFL,P51X,HFLUX,0.014
!*
FLST,2,2,4,ORDE,2
FITEM,2,1
FITEM,2,-2
/GO
!*
!*BOTTOM HEAD
SFL,P51X,HFLUX,0.0065,
SFL,P51X,HFLUX,0.0065
!*
FLST,2,3,4,ORDE,3
FITEM,2,8
FITEM,2,16
FITEM,2,35
/GO
!*
!*WALL
SFL,P51X,HFLUX,0.007,
SFL,P51X,HFLUX,0.007
!*
```

```
FLST,2,10,4,ORDE,10
FITEM,2,21
FITEM,2,24
FITEM,2,31
FITEM,2,48
FITEM,2,55
FITEM,2,60
FITEM,2,63
FITEM,2,-64
FITEM,2,66
FITEM,2,-67
/GO
!*
!*CLAMP
SFL,P51X,HFLUX,0.0065,
SFL,P51X,HFLUX,0.0065
!*
/REPLOT,RESIZE
/REPLOT,RESIZE
FLST,5,7,2,ORDE,4
FITEM,5,1064
FITEM,5,-1068
FITEM,5,1089
FITEM,5,-1090
CM,_Y,ELEM
ESEL, , , ,P51X
CM,_Y1,ELEM
CMSEL,S,_Y
CMDELE,_Y
!*
/GO
!*
!*HEAD & FLANGE OD
SFE,_Y1,2,HFLUX, ,0.007, , ,
CMDELE,_Y1
TIME,500
AUTOTS,-1
DELTIM, ,1,700,1
KBC,1
TSRES,ERASE
LSWRITE,1,
!*
TIME,1000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,2,
!*
TIME,2000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,3,
!*
TIME,4000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,4,
!*
TIME,6000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,5,
!*
TIME,8000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,6,
!*
TIME,10000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,7,
!*
TIME,12000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,8,
!*
TIME,14000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,9,
!*
TIME,16000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,10,
!*
TIME,18000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,11,
!*
SFLDELE,ALL,ALL
FLST,2,7,2,ORDE,4
FITEM,2,1057
FITEM,2,-1061
FITEM,2,1082
FITEM,2,-1083
```

```
SFEDELE,P51X,all,HFLUX
TIME,19800
AUTOTS,-1
KBC,1
TSRES,ERASE
LSWRITE,12,
```

8.7 Large Vessel Stress Analysis – Heatup Transient

```
/PREP7
/TITLE, BATCH SCWO PHASE 3 STRESS
ANALYSIS
!*
ET,1,PLANE55
!*
KEYOPT,1,1,0
KEYOPT,1,3,1
KEYOPT,1,4,0
KEYOPT,1,8,0
KEYOPT,1,9,0
!*
MPTEMP,1,78,200,400,600,800,1000,
MPTEMP,7,1200, , , , , ,
MPDATA,KXX,1,1,1.813e-4,1.948e-
4,2.180e-4,2.411e-4,2.643e-
4,2.874e-4,
MPDATA,KXX,1,7,3.106e-4, , , , , ,
MPDATA,ALPX,1,1,0.0,6.4e-6,7.0e-
6,7.4e-6,7.6e-6,7.7e-6,
MPDATA,ALPX,1,7,8.0e-6, , , , , ,
MPDATA,C,1,1,.1,.104,.111,.117,.12
4,.131,
MPDATA,C,1,7,.137, , , , , ,
MPDATA,DENS,1,1,0.302,0.302,0.302,
0.302,0.302,0.302,
MPDATA,DENS,1,7,0.302, , , , , ,
MPDATA,EX,1,1,30.6e6,30.0e6,29.0e6
,28.0e6,26.9e6,25.8e6,
MPDATA,EX,1,7,24.6e6, , , , , ,
MPDATA,GXY,1,1,11.8e6,11.6e6,11.2e
6,10.8e6,10.4e6,9.9e6,
MPDATA,GXY,1,7,9.5e6, , , , , ,
MPDATA,PRXY,1,1,0.3,0.3,0.3,0.3,0.
3,0.3,
MPDATA,PRXY,1,7,0.3, , , , , ,
!*
K,1,0,0
K,2,10.0
K,3,13.875
K,4,,6.375,,
LSTR,       1,       2
LSTR,       2,       3
LSTR,       1,       4
FLST,2,2,4,ORDE,2
FITEM,2,1
FITEM,2,-2
ADRAG,P51X, , , , , ,       3
K,8,10.0,74.375,,
K,9,10.0,82.75,,
K,10,10.0,84.375,,
K,11,10.0,86.0
K,12,10.0,92.375
LSTR,       6,       8
LSTR,       8,       9
LSTR,       9,      10
LSTR,      10,      11
LSTR,      11,      12
FLST,8,5,4
FITEM,8,9
FITEM,8,10
FITEM,8,11
FITEM,8,12
FITEM,8,13
ADRAG,       7, , , , ,P51X
K,23,0,84.375
LSTR,      10,      23
FLST,2,2,4,ORDE,2
FITEM,2,12
FITEM,2,-13
ADRAG,P51X, , , , , ,      29
K,27,14.625,74.375,,
LSTR,      14,      27
FLST,2,4,4,ORDE,4
FITEM,2,19
FITEM,2,22
FITEM,2,25
FITEM,2,28
ADRAG,P51X, , , , , ,      35
K,33,15.625,84.375,,
```

```
LSTR,      30,      33
FLST,2,2,4,ORDE,2
FITEM,2,39
FITEM,2,41
ADRAG,P51X, , , , , ,      45
NUMMRG,KP,.1, ,
K,37,15.625,86.25,,
K,38,15.625,90.71875,,
K,39,21.25,84.375,,
LSTR,      36,      37
LSTR,      37,      38
LSTR,      33,      39
FLST,2,3,4,ORDE,3
FITEM,2,5
FITEM,2,15
FITEM,2,49
ADRAG,P51X, , , , , ,      18
K,40,14.9685,86.25,,
LSTR,      37,      40
ADRAG,      15, , , , , ,      52
K,41,15.625,82.5,,
K,42,15.625,78.03125,,
LSTR,      34,      41
LSTR,      41,      42
FLST,8,3,4
FITEM,8,46
FITEM,8,56
FITEM,8,57
ADRAG,      18, , , , , ,P51X
K,46,14.9685,78.03125,,
LSTR,      42,      46
ADRAG,      57, , , , , ,      67
NUMMRG,KP,0.1, ,
FLST,2,3,5,ORDE,2
FITEM,2,1
FITEM,2,-3
ADELE,P51X
LPLOT
!*
LFILLT,9,4,1.0, ,
FLST,2,4,3
FITEM,2,39
FITEM,2,4
FITEM,2,1
FITEM,2,2
A,P51X
FLST,2,5,3
FITEM,2,34
FITEM,2,39
FITEM,2,2
FITEM,2,3
FITEM,2,7
A,P51X
FLST,2,4,3
FITEM,2,8
FITEM,2,34
FITEM,2,7
FITEM,2,14
A,P51X
APLOT
NUMMRG,KP,0.2, ,
AATT,       1, ,   1,       0
ESIZE,0.75,0,
MSHKEY,0
FLST,5,23,5,ORDE,2
FITEM,5,1
FITEM,5,-23
CM,_Y,AREA
ASEL, , , ,P51X
CM,_Y1,AREA
CHKMSH,'AREA'
CMSEL,S,_Y
!*
AMESH,_Y1
!*
CMDEL,_Y
CMDEL,_Y1
CMDEL,_Y2
!*
ETCHG,TTS
!*
KEYOPT,1,1,0
KEYOPT,1,2,0
KEYOPT,1,3,1
KEYOPT,1,5,0
KEYOPT,1,6,0
!*
ANTYPE,0
FLST,2,1,1,ORDE,1
FITEM,2,14
!*
/GO
D,P51X, ,0.0, , , ,UY, , , , ,
!*
/TITLE, BATCH SCWO LARGE VESSEL
HEATUP 500 SEC
LDREAD,TEMP,,,500, ,LHeatR,rth,
LSWRITE,1,
!*
/TITLE, BATCH SCWO LARGE VESSEL
HEATUP 1000 SEC
LDREAD,TEMP,,,1000, ,LHeatR,rth,
LSWRITE,2,
!*
/TITLE, BATCH SCWO LARGE VESSEL
HEATUP 2000 SEC
LDREAD,TEMP,,,2000, ,LHeatR,rth,
LSWRITE,3,
```

```
!*
/TITLE, BATCH SCWO LARGE VESSEL
HEATUP 4000 SEC
LDREAD,TEMP,,,4000, ,LHeatR,rth,
LSWRITE,4,
!*
/TITLE, BATCH SCWO LARGE VESSEL
HEATUP 6000 SEC
LDREAD,TEMP,,,6000, ,LHeatR,rth,
LSWRITE,5,
!*
/TITLE, BATCH SCWO LARGE VESSEL
HEATUP 8000 SEC
LDREAD,TEMP,,,8000, ,LHeatR,rth,
LSWRITE,6,
!*
/TITLE, BATCH SCWO LARGE VESSEL
HEATUP 10000 SEC
LDREAD,TEMP,,,10000, ,LHeatR,rth,
LSWRITE,7,
!*
/TITLE, BATCH SCWO LARGE VESSEL
HEATUP 12000 SEC
LDREAD,TEMP,,,12000, ,LHeatR,rth,
LSWRITE,8,
!*
/TITLE, BATCH SCWO LARGE VESSEL
HEATUP 14000 SEC
LDREAD,TEMP,,,14000, ,LHeatR,rth,
LSWRITE,9,
!*
/TITLE, BATCH SCWO LARGE VESSEL
HEATUP 16000 SEC
LDREAD,TEMP,,,16000, ,LHeatR,rth,
LSWRITE,10,
!*
/TITLE, BATCH SCWO LARGE VESSEL
HEATUP 18000 SEC
LDREAD,TEMP,,,18000, ,LHeatR,rth,
LSWRITE,11,
!*
/TITLE, BATCH SCWO LARGE VESSEL
HEATUP 19800 SEC
LDREAD,TEMP,,,19800, ,LHeatR,rth,
LSWRITE,12,
!*
```

8.8 Large Vessel Thermal Analysis – Cooldown Transient

```
/PREP7
/TITLE, BATCH SCWO PHASE 3 THERMAL
ANALYSIS
!*
ET,1,PLANE55
!*
KEYOPT,1,1,0
KEYOPT,1,3,1
KEYOPT,1,4,0
KEYOPT,1,8,0
KEYOPT,1,9,0
!*
MPTEMP,1,78,200,400,600,800,1000,
MPTEMP,7,1200, , , , , ,
MPDATA,KXX,1,1,1.813e-4,1.948e-
4,2.180e-4,2.411e-4,2.643e-
4,2.874e-4,
MPDATA,KXX,1,7,3.106e-4, , , , , ,
MPDATA,ALPX,1,1,0.0,6.4e-6,7.0e-
6,7.4e-6,7.6e-6,7.7e-6,
MPDATA,ALPX,1,7,8.0e-6, , , , , ,
MPDATA,C,1,1,.1,.104,.111,.117,.12
4,.131,
MPDATA,C,1,7,.137, , , , , ,
MPDATA,DENS,1,1,0.302,0.302,0.302,
0.302,0.302,0.302,
MPDATA,DENS,1,7,0.302, , , , , ,
MPDATA,EX,1,1,30.6e6,30.0e6,29.0e6
,28.0e6,26.9e6,25.8e6,
MPDATA,EX,1,7,24.6e6, , , , , ,
MPDATA,GXY,1,1,11.8e6,11.6e6,11.2e
6,10.8e6,10.4e6,9.9e6,
MPDATA,GXY,1,7,9.5e6, , , , , ,
MPDATA,PRXY,1,1,0.3,0.3,0.3,0.3,0.
3,0.3,
MPDATA,PRXY,1,7,0.3, , , , , ,
!*
K,1,0,0
K,2,10.0
K,3,13.875
K,4,,6.375,,
LSTR,       1,       2
LSTR,       2,       3
LSTR,       1,       4
FLST,2,2,4,ORDE,2
FITEM,2,1
FITEM,2,-2
ADRAG,P51X, , , , , ,       3
```

```
K,8,10.0,74.375,,
K,9,10.0,82.75,,
K,10,10.0,84.375,,
K,11,10.0,86.0
K,12,10.0,92.375
LSTR,       6,       8
LSTR,       8,       9
LSTR,       9,      10
LSTR,      10,      11
LSTR,      11,      12
FLST,8,5,4
FITEM,8,9
FITEM,8,10
FITEM,8,11
FITEM,8,12
FITEM,8,13
ADRAG,       7, , , , , ,P51X
K,23,0,84.375
LSTR,      10,      23
FLST,2,2,4,ORDE,2
FITEM,2,12
FITEM,2,-13
ADRAG,P51X, , , , , ,      29
K,27,14.625,74.375,,
LSTR,      14,      27
FLST,2,4,4,ORDE,4
FITEM,2,19
FITEM,2,22
FITEM,2,25
FITEM,2,28
ADRAG,P51X, , , , , ,      35
K,33,15.625,84.375,,
LSTR,      30,      33
FLST,2,2,4,ORDE,2
FITEM,2,39
FITEM,2,41
ADRAG,P51X, , , , , ,      45
NUMMRG,KP,.1, ,
K,37,15.625,86.25,,
K,38,15.625,90.71875,,
K,39,21.25,84.375,,
LSTR,      36,      37
LSTR,      37,      38
LSTR,      33,      39
FLST,2,3,4,ORDE,3
FITEM,2,5
FITEM,2,15
FITEM,2,49
ADRAG,P51X, , , , , ,      18
K,40,14.9685,86.25,,
LSTR,      37,      40
ADRAG,      15, , , , , ,      52
K,41,15.625,82.5,,
K,42,15.625,78.03125,,
LSTR,      34,      41
LSTR,      41,      42
FLST,8,3,4
FITEM,8,46
FITEM,8,56
FITEM,8,57
ADRAG,      18, , , , , ,P51X
K,46,14.9685,78.03125,,
LSTR,      42,      46
ADRAG,      57, , , , , ,      67
NUMMRG,KP,0.1, ,
FLST,2,3,5,ORDE,2
FITEM,2,1
FITEM,2,-3
ADELE,P51X
LPLOT
!*
LFILLT,9,4,1.0, ,
FLST,2,4,3
FITEM,2,39
FITEM,2,4
FITEM,2,1
FITEM,2,2
A,P51X
FLST,2,5,3
FITEM,2,34
FITEM,2,39
FITEM,2,2
FITEM,2,3
FITEM,2,7
A,P51X
FLST,2,4,3
FITEM,2,8
FITEM,2,34
FITEM,2,7
FITEM,2,14
A,P51X
APLOT
NUMMRG,KP,0.2, ,
AATT,       1, ,   1,       0
ESIZE,0.75,0,
MSHKEY,0
FLST,5,23,5,ORDE,2
FITEM,5,1
FITEM,5,-23
CM,_Y,AREA
ASEL, , , ,P51X
CM,_Y1,AREA
CHKMSH,'AREA'
CMSEL,S,_Y
!*
AMESH,_Y1
!*
CMDEL,_Y
```

```
CMDEL,_Y1
CMDEL,_Y2
ANTYPE,4
!*
TUNIF,1200.
!*
FLST,2,18,4,ORDE,18
FITEM,2,1
FITEM,2,-2
FITEM,2,8
FITEM,2,16
FITEM,2,21
FITEM,2,24
FITEM,2,26
FITEM,2,31
FITEM,2,34
FITEM,2,-35
FITEM,2,44
FITEM,2,48
FITEM,2,55
FITEM,2,60
FITEM,2,63
FITEM,2,-64
FITEM,2,66
FITEM,2,-67
/GO
!*
SFL,P51X,CONV,1.35e-5, ,70,
FLST,5,7,2,ORDE,4
FITEM,5,1064
FITEM,5,-1068
FITEM,5,1089
FITEM,5,-1090
CM,_Y,ELEM
ESEL, , , ,P51X
CM,_Y1,ELEM
CMSEL,S,_Y
CMDELE,_Y
!*
/GO
!*
SFE,_Y1,2,CONV, ,1.35e-5
SFE,_Y1,2,CONV,2,70.0
!*
TIME,1000
AUTOTS,-1
DELTIM, ,1,1000,1
KBC,1
TSRES,ERASE
LSWRITE,1,
!*
TIME,2000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,2,
!*
TIME,4000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,3,
!*
TIME,8000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,4,
!*
TIME,16000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,5,
!*
TIME,32000
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,6,
!*
TIME,43200
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,7,
!*
TIME,46800
AUTOTS,-1
KBC,0
TSRES,ERASE
LSWRITE,8,
```

8.9 Large Vessel Stress Analysis – Cooldown Transient

```
/PREP7
```

```
/TITLE, BATCH SCWO PHASE 3 STRESS
ANALYSIS
!*
ET,1,PLANE55
!*
KEYOPT,1,1,0
KEYOPT,1,3,1
KEYOPT,1,4,0
KEYOPT,1,8,0
KEYOPT,1,9,0
!*
MPTEMP,1,78,200,400,600,800,1000,
MPTEMP,7,1200, , , , , ,
MPDATA,KXX,1,1,1.813e-4,1.948e-
4,2.180e-4,2.411e-4,2.643e-
4,2.874e-4,
MPDATA,KXX,1,7,3.106e-4, , , , , ,
MPDATA,ALPX,1,1,0.0,6.4e-6,7.0e-
6,7.4e-6,7.6e-6,7.7e-6,
MPDATA,ALPX,1,7,8.0e-6, , , , , ,
MPDATA,C,1,1,.1,.104,.111,.117,.12
4,.131,
MPDATA,C,1,7,.137, , , , , ,
MPDATA,DENS,1,1,0.302,0.302,0.302,
0.302,0.302,0.302,
MPDATA,DENS,1,7,0.302, , , , , ,
MPDATA,EX,1,1,30.6e6,30.0e6,29.0e6
,28.0e6,26.9e6,25.8e6,
MPDATA,EX,1,7,24.6e6, , , , , ,
MPDATA,GXY,1,1,11.8e6,11.6e6,11.2e
6,10.8e6,10.4e6,9.9e6,
MPDATA,GXY,1,7,9.5e6, , , , , ,
MPDATA,PRXY,1,1,0.3,0.3,0.3,0.3,0.
3,0.3,
MPDATA,PRXY,1,7,0.3, , , , , ,
!*
K,1,0,0
K,2,10.0
K,3,13.875
K,4,,6.375,,
LSTR,       1,       2
LSTR,       2,       3
LSTR,       1,       4
FLST,2,2,4,ORDE,2
FITEM,2,1
FITEM,2,-2
ADRAG,P51X, , , , , ,       3
K,8,10.0,74.375,,
K,9,10.0,82.75,,
K,10,10.0,84.375,,
K,11,10.0,86.0
K,12,10.0,92.375
LSTR,       6,       8
LSTR,       8,       9
LSTR,       9,      10
LSTR,      10,      11
LSTR,      11,      12
FLST,8,5,4
FITEM,8,9
FITEM,8,10
FITEM,8,11
FITEM,8,12
FITEM,8,13
ADRAG,       7, , , , , ,P51X
K,23,0,84.375
LSTR,      10,      23
FLST,2,2,4,ORDE,2
FITEM,2,12
FITEM,2,-13
ADRAG,P51X, , , , , ,      29
K,27,14.625,74.375,,
LSTR,      14,      27
FLST,2,4,4,ORDE,4
FITEM,2,19
FITEM,2,22
FITEM,2,25
FITEM,2,28
ADRAG,P51X, , , , , ,      35
K,33,15.625,84.375,,
LSTR,      30,      33
FLST,2,2,4,ORDE,2
FITEM,2,39
FITEM,2,41
ADRAG,P51X, , , , , ,      45
NUMMRG,KP,.1, ,
K,37,15.625,86.25,,
K,38,15.625,90.71875,,
K,39,21.25,84.375,,
LSTR,      36,      37
LSTR,      37,      38
LSTR,      33,      39
FLST,2,3,4,ORDE,3
FITEM,2,5
FITEM,2,15
FITEM,2,49
ADRAG,P51X, , , , , ,      18
K,40,14.9685,86.25,,
LSTR,      37,      40
ADRAG,      15, , , , , ,      52
K,41,15.625,82.5,,
K,42,15.625,78.03125,,
LSTR,      34,      41
LSTR,      41,      42
FLST,8,3,4
FITEM,8,46
FITEM,8,56
FITEM,8,57
ADRAG,      18, , , , , ,P51X
```

```
K,46,14.9685,78.03125,,
LSTR,       42,       46
ADRAG,       57, , , , , ,       67
NUMMRG,KP,0.1, ,
FLST,2,3,5,ORDE,2
FITEM,2,1
FITEM,2,-3
ADELE,P51X
LPLOT
!*
LFILLT,9,4,1.0, ,
FLST,2,4,3
FITEM,2,39
FITEM,2,4
FITEM,2,1
FITEM,2,2
A,P51X
FLST,2,5,3
FITEM,2,34
FITEM,2,39
FITEM,2,2
FITEM,2,3
FITEM,2,7
A,P51X
FLST,2,4,3
FITEM,2,8
FITEM,2,34
FITEM,2,7
FITEM,2,14
A,P51X
APLOT
NUMMRG,KP,0.2, ,
AATT,        1, ,   1,        0
ESIZE,0.75,0,
MSHKEY,0
FLST,5,23,5,ORDE,2
FITEM,5,1
FITEM,5,-23
CM,_Y,AREA
ASEL, , , ,P51X
CM,_Y1,AREA
CHKMSH,'AREA'
CMSEL,S,_Y
!*
AMESH,_Y1
!*
CMDEL,_Y
CMDEL,_Y1
CMDEL,_Y2
!*
ETCHG,TTS
!*
KEYOPT,1,1,0
KEYOPT,1,2,0
KEYOPT,1,3,1
KEYOPT,1,5,0
KEYOPT,1,6,0
!*
ANTYPE,0
FLST,2,1,1,ORDE,1
FITEM,2,14
!*
/GO
D,P51X, ,0.0, , , ,UY, , , , ,
!*
/TITLE, BATCH SCWO LARGE VESSEL
Cooldown 1000 SEC
LDREAD,TEMP,,,1000, ,LCoolR,rth,
LSWRITE,1,
!*
/TITLE, BATCH SCWO LARGE VESSEL
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LSWRITE,2,
!*
/TITLE, BATCH SCWO LARGE VESSEL
Cooldown 4000 SEC
LDREAD,TEMP,,,4000, ,LCoolR,rth,
LSWRITE,3,
!*
/TITLE, BATCH SCWO LARGE VESSEL
Cooldown 8000 SEC
LDREAD,TEMP,,,8000, ,LCoolR,rth,
LSWRITE,4,
!*
/TITLE, BATCH SCWO LARGE VESSEL
Cooldown 16000 SEC
LDREAD,TEMP,,,16000, ,LCoolR,rth,
LSWRITE,5,
!*
/TITLE, BATCH SCWO LARGE VESSEL
Cooldown 32000 SEC
LDREAD,TEMP,,,32000, ,LCoolR,rth,
LSWRITE,6,
!*
/TITLE, BATCH SCWO LARGE VESSEL
Cooldown 43200 SEC
LDREAD,TEMP,,,43200, ,LCoolR,rth,
LSWRITE,7,
!*
/TITLE, BATCH SCWO LARGE VESSEL
Cooldown 46800 SEC
LDREAD,TEMP,,,46800, ,LCoolR,rth,
LSWRITE,8,
!*
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8.10 Large Vessel Stress Analysis – Pressure

```
/PREP7
/TITLE, BATCH SCWO PHASE 3 STRESS
ANALYSIS
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ET,1,PLANE55
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KEYOPT,1,3,1
KEYOPT,1,4,0
KEYOPT,1,8,0
KEYOPT,1,9,0
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MPTEMP,7,1200, , , , , ,
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4,2.180e-4,2.411e-4,2.643e-
4,2.874e-4,
MPDATA,KXX,1,7,3.106e-4, , , , , ,
MPDATA,ALPX,1,1,0.0,6.4e-6,7.0e-
6,7.4e-6,7.6e-6,7.7e-6,
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4,.131,
MPDATA,C,1,7,.137, , , , , ,
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0.302,0.302,0.302,
MPDATA,DENS,1,7,0.302, , , , , ,
MPDATA,EX,1,1,30.6e6,30.0e6,29.0e6
,28.0e6,26.9e6,25.8e6,
MPDATA,EX,1,7,24.6e6, , , , , ,
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MPDATA,GXY,1,7,9.5e6, , , , , ,
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3,0.3,
MPDATA,PRXY,1,7,0.3, , , , , ,
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K,2,10.0
K,3,13.875
K,4,,6.375,,
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LSTR,       2,       3
LSTR,       1,       4
FLST,2,2,4,ORDE,2
FITEM,2,1
FITEM,2,-2
ADRAG,P51X, , , , , ,       3
K,8,10.0,74.375,,
K,9,10.0,82.75,,
K,10,10.0,84.375,,
K,11,10.0,86.0
K,12,10.0,92.375
LSTR,       6,       8
LSTR,       8,       9
LSTR,       9,      10
LSTR,      10,      11
LSTR,      11,      12
FLST,8,5,4
FITEM,8,9
FITEM,8,10
FITEM,8,11
FITEM,8,12
FITEM,8,13
ADRAG,       7, , , , , ,P51X
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LSTR,      10,      23
FLST,2,2,4,ORDE,2
FITEM,2,12
FITEM,2,-13
ADRAG,P51X, , , , , ,      29
K,27,14.625,74.375,,
LSTR,      14,      27
FLST,2,4,4,ORDE,4
FITEM,2,19
FITEM,2,22
FITEM,2,25
FITEM,2,28
ADRAG,P51X, , , , , ,      35
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NUMMRG,KP,.1, ,
K,37,15.625,86.25,,
K,38,15.625,90.71875,,
K,39,21.25,84.375,,
LSTR,      36,      37
LSTR,      37,      38
LSTR,      33,      39
FLST,2,3,4,ORDE,3
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FITEM,2,15
FITEM,2,49
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ADRAG,      15, , , , , ,      52
K,41,15.625,82.5,,
K,42,15.625,78.03125,,
LSTR,      34,      41
LSTR,      41,      42
FLST,8,3,4
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FITEM,8,56
FITEM,8,57
ADRAG,      18, , , , , ,P51X
K,46,14.9685,78.03125,,
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ADRAG,      57, , , , , ,      67
NUMMRG,KP,0.1, ,
FLST,2,3,5,ORDE,2
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FITEM,2,-3
ADELE,P51X
LPLOT
!*
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FITEM,2,4
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FITEM,2,2
A,P51X
FLST,2,5,3
FITEM,2,34
FITEM,2,39
FITEM,2,2
FITEM,2,3
FITEM,2,7
A,P51X
FLST,2,4,3
FITEM,2,8
FITEM,2,34
FITEM,2,7
FITEM,2,14
A,P51X
APLOT
NUMMRG,KP,0.2, ,
AATT,       1, ,   1,       0
ESIZE,0.75,0,
MSHKEY,0
FLST,5,23,5,ORDE,2
FITEM,5,1
FITEM,5,-23
CM,_Y,AREA
ASEL, , , ,P51X
CM,_Y1,AREA
CHKMSH,'AREA'
CMSEL,S,_Y
!*
AMESH,_Y1
!*
CMDEL,_Y
CMDEL,_Y1
CMDEL,_Y2
!*
ETCHG,TTS
!*
KEYOPT,1,1,0
KEYOPT,1,2,0
KEYOPT,1,3,1
KEYOPT,1,5,0
KEYOPT,1,6,0
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ANTYPE,0
TUNIF,1200.
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/REPLOT,RESIZE
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FITEM,2,9
FITEM,2,-11
FITEM,2,29
FITEM,2,51
/GO
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SFL,P51X,PRES,4000.0,
/TITLE, BATCH SCWO LARGE VESSEL
4000 PRESSURE
LSWRITE,1
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ATTACHMENT A

REFLANGE G-CON CATALOG DATA

G-CON® Buttweld Hubs

The **Reflange** Standard Buttweld hub materials are A-105 Carbon Steel and A 182-F316 Stainless Steel. **Reflange** also offers hubs in a wide variety of materials including MONEL*, INCONEL*, low alloy, austenitic stainless steels, and all of the carbon, titanium and zirconium alloys.

Sealing surfaces on carbon steel and low alloy steel hubs and fittings are protected by electroless nickel coating.

The welding bevel and part tolerances are in accordance with ANSI B16.5.

*MONEL and INCONEL are trademarks of International Nickel Co.

PIPE SIZE	PIPE SCH.	G-CON® B.W. HUB PART No.	APPROX. Wt. (lbs.)	G-CON® SEAL PART No.	G-CON® CLAMP PART No.	DIMENSIONS (inches)					
						PIPE O.D. A	PIPE I.D. B	C	D*1	E	F
1/2	80	FN.5008 G05	1	G05	C-0075	0.840	0.546	1.562	1.500	1.063	0.133
1/2	80	F.5008 G05	3	G05	C-01	0.840	0.546	2.000	1.750	1.500	0.313
3/4	160	FN.7516 G05	1	G05	C-0075	1.050	0.614	1.562	1.500	1.063	0.133
3/4	160	F.7516 G05	3	G05	C-01	1.050	0.614	2.000	1.750	1.500	0.313
1	40	F0104 G11	3	G11	C-01	1.315	1.049	2.000	1.750	1.500	0.313
	80	F0108 G11	3	G11	C-01	1.315	0.957	2.000	1.750	1.500	0.313
	160	F0116 G07	3	G07	C-01	1.315	0.815	2.000	1.750	1.500	0.313
	XX	F01XX G05	3	G05	C-01	1.315	0.599	2.000	1.750	1.500	0.313
1-1/2	40	F1.504 G14	3	G14	C-1.5	1.900	1.610	3.125	2.375	2.375	0.437
	80	F1.508 G14	3	G14	C-1.5	1.900	1.500	3.125	2.375	2.375	0.437
	160	F1.516 G14	3	G14	C-1.5	1.900	1.338	3.125	2.375	2.375	0.437
	XX	F1.5XX G11	3	G11	C-1.5	1.900	1.100	3.125	2.375	2.375	0.500
	...*1	F1.5- 497 G07	3	G07	C-1.5	1.900	0.906	3.125	2.438	2.375	0.559
2	40	F0204 G20	3	G20	C-02	2.375	2.063	3.625	2.750	2.875	0.437
	80	F0208 G20	3	G20	C-02	2.375	1.939	3.625	2.750	2.875	0.437
	160	F0216 G20	3	G20	C-02	2.375	1.689	3.625	2.750	2.875	0.437
	XX	F02XX G14	3	G14	C-02	2.375	1.503	3.625	2.750	2.875	0.437
	...*1	F02- 625 G11	4	G11	C-02	2.375	1.125	3.625	2.812	2.875	0.558
2-1/2	40	F2.504 G25	6	G25	C-03	2.875	2.469	5.000	3.250	4.000	0.500
	80	F2.508 G25	6	G25	C-03	2.875	2.323	5.000	3.250	4.000	0.500
	160	F2.516 G20	7	G20	C-03	2.875	2.125	5.000	3.250	4.000	0.500
	XX	F2.5XX G20	7	G20	C-03	2.875	1.771	5.000	3.250	4.000	0.500
	...*1	F2.5- 633 G14	7	G14	C-03	2.875	1.510	5.000	3.375	4.000	0.625
3	40	F0304 G27	5	G27	C-03	3.500	3.063	5.000	3.250	4.000	0.500
	80	F0308 G27	5	G27	C-03	3.500	2.900	5.000	3.250	4.000	0.500
	160	F0316 G25	7	G25	C-03	3.500	2.624	5.000	3.250	4.000	0.500
	XX	F03XX G23	8	G23	C-03	3.500	2.300	5.000	3.250	4.000	0.500
	...*1	F03- 719 G20	9	G20	C-03	3.500	2.063	5.000	3.250	4.000	0.500
4	40	F0404 G40	8	G40	C-04	4.500	4.026	6.000	3.625	5.000	0.500
	80	F0408 G40	8	G40	C-04	4.500	3.826	6.000	3.625	5.000	0.500
	160	F0416 G34	11	G34	C-04	4.500	3.438	6.000	3.625	5.000	0.500
	XX	F04XX G31	12	G31	C-04	4.500	3.152	6.000	3.625	5.000	0.500
	...*1	F04- 914 G25	15	G25	C-04	4.500	2.672	6.000	3.625	5.000	0.500

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G-CON® Buttweld Hubs

PIPE SIZE	PIPE SCH.	G-CON® B.W. HUB PART No.	APPROX. Wt. (lbs.)	G-CON® SEAL PART No.	G-CON® CLAMP PART No.	DIMENSIONS (inches)					
						PIPE O.D. A	PIPE I.D. B	C	D*3	E	F
5	40	F0504 G52	11	G52	C-05	5.563	5.047	7.500	4.375	6.500	0.625
	80	F0508 G52	11	G52	C-05	5.563	4.813	7.500	4.375	6.500	0.625
	160	F0516 G46	17	G46	C-05	5.563	4.313	7.500	4.375	6.500	0.625
	XX	F05XX G40	24	G40	C-05	5.563	4.063	7.500	4.375	6.500	0.625
	...*1	F05-.938 G34	24	G34	C-05	5.563	3.688	7.500	4.375	6.500	0.625
6	40	F0604 G62	22	G62	C-06	6.625	6.063	9.250	4.625	7.750	0.750
	80	F0608 G62	22	G62	C-06	6.625	5.761	9.250	4.625	7.750	0.750
	160	F0616 G52	31	G52	C-06	6.625	5.189	9.250	4.625	7.750	0.812
	XX	F06XX G52	31	G52	C-06	6.625	4.897	9.250	4.625	7.750	0.812
	...*1	F06-.938 G46	37	G46	C-06	6.625	4.750	9.250	4.750	7.750	0.934
8	40	F0804 G82	32	G82	C-X8	8.625	7.981	11.500	5.375	10.000	0.750
	80	F0808 G76	41	G76	C-X8	8.625	7.625	11.500	5.375	10.000	0.750
	160	F0816 G72	50	G72	C-X8	8.625	6.813	11.500	5.375	10.000	0.750
	XX	F08XX G72	50	G72	C-X8	8.625	6.875	11.500	5.375	10.000	0.750
	...*1	F08-1.656 G52	78	G52	C-X8	8.625	5.313	11.500	5.500	10.000	0.934
10	40	F1004 G102	55	G102	C-X10H	10.750	10.020	13.625	6.000	11.625	1.250
	80	F1008 G97	55	G97	C-X10H	10.750	9.564	13.625	6.000	11.625	1.250
	160	F1016 G84	89	G84	C-X10H	10.750	8.500	13.625	6.000	11.625	1.250
	...*1	F10-1.500 G76	115	G76	C-X10H	10.750	7.750	13.625	6.000	11.625	1.250
12	80	F1208 G112	98	G112	C-X12M	12.750	11.375	16.000	6.625	14.000	1.250
	160	F1216 G102	129	G102	C-X12M	12.750	10.125	16.000	6.625	14.000	1.375
	...*1	F12-1.625 G94	140	G94	C-X12M	12.750	9.500	16.000	6.625	14.000	1.375
16	160	F1616 G130	118	G130	C-X16	16.000	*12.814	19.500	7.750	18.000	.750
	...*1	F16-2.000 G120	122	G120	C-X16	16.000	12.000	19.500	7.750	18.000	.750
18	160	F1816 G144	170	G144	C-X18	18.000	14.438	21.750	8.250	20.250	.750
	...*1	F18-2.063 G137	174	G137	C-X18	18.000	13.875	21.750	8.250	20.250	.750
24	160	F2416 G192	300	G192	C-24	24.000	19.314	29.500	9.750	27.500	1.000
	...*1	F24-3.500 G170	310	G170	C-24	24.000	17.000	29.500	9.750	27.500	1.000
36	...*1	F36 G304	1400	G304	C-36	36.000	30.500	41.000	12.000	38.500	1.306

G-CON® Heavy Duty Buttweld Hubs

PIPE SIZE	PIPE SCH.	G-CON® B.W. HUB PART No.	APPROX. Wt. (lbs.)	G-CON® SEAL PART No.	G-CON® CLAMP PART No.	DIMENSIONS (inches)					
						PIPE O.D. A	PIPE I.D. B	C	D*3	E	F
2*2	XX	FB-02XX G14	10	G14	C-B	2.375	1.503	4.750	3.250	3.750	0.625
	...*1	FB-02-1.125 G11	11	G11	C-B	2.375	1.125	4.750	3.250	3.750	0.687
3*2	XX	FC-03XX G23	14	G23	C-C	3.500	2.300	5.500	3.500	4.500	0.625
	...*1	FC-03-.719 G20	16	G20	C-C	3.500	2.063	5.500	3.500	4.500	0.625
4*2	XX	FD-04XX G31	23	G31	C-D	4.500	31.52	6.750	4.000	5.750	0.625
	...*1	FD-04-.914 G25	26	G25	C-D	4.500	2.672	6.750	4.000	5.750	0.625
14*2	80	FP-1408 G120	153	G120	C-P	14.000	12.500	18.500	7.250	16.500	1.250
	...*1	FP-14-1.875 G102	200	G102	C-P	14.000	10.250	18.500	7.250	16.500	1.250
16*2	STD	FS-1657 G152	194	G152	C-S	16.000	15.250	21.000	7.875	19.000	1.687
	...*1	FS-16-1.250 G134	251	G134	C-S	16.000	13.500	21.000	7.875	19.000	1.687
20*2	80	FU-2008 G180	331	G180	C-U	20.000	17.938	25.000	8.750	23.000	1.625
	...*1	FU-20-2.375 G152	437	G152	C-U	20.000	15.250	25.000	8.750	23.000	1.625
24*2	160	FV-2416 G200	300	G200	C-5V	24.000	19.314	26.000	9.000	24.000	1.250
	...*1	FV-24-3.500 G170	385	G170	C-5V	24.000	17.000	26.000	9.000	24.000	1.500
24*2	80	FY-2408 G220	567	G220	C-3Y	24.000	21.564	31.250	10.000	28.250	1.625
	...*1	FY-24-1.500 G210	622	G210	C-3Y	24.000	21.000	31.250	10.000	28.250	1.625

Note:
All dimensions are for reference only.
*1 This is not a Standard Pipe Schedule.
*2 These are the nominal pipe sizes typically associated with these connections although other pipe sizes and schedules can be accommodated.
*3 Length of hub may increase when used with wall thicknesses greater than standard pipe schedules.

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G-CON® Blind Hubs

G-CON® blind hubs are available for standard sized G-CON® connections. Because they are designed to carry the full basic pressure rating of the G-CON® connection, they may be used as closures for pressure vessels and heat exchangers.

Blind hubs may be drilled and tapped for instrumentation or otherwise customized to fit specific requirements.

PIPE SIZE	PIPE SCH.	G-CON B. W. HUB No.	APPROX. Wt. (lbs.)	G-CON SEAL PART No.	CLAMP No.	DIMENSIONS (inches)				
						C	D	E	F	G
1/2	80	BN.50 G05	.5	G05	C-0075	1.562	1.5	1.063	0.133	.135
1/2	80	B.50 G05	3	G05	C-01	2.000	1.750	1.500	0.313	.135
3/4	160	BN.75 G05	.5	G05	C-0075	1.562	1.5	1.063	0.133	.135
3/4	160	B.75 G05	3	G05	C-01	2.000	1.750	1.500	0.313	.135
1	40	B01 G11	3	G11	C-01	2.000	1.750	1.500	0.313	.135
	80	B01 G11	3	G11	C-01	2.000	1.750	1.500	0.313	.135
	160	B01 G07	3	G07	C-01	2.000	1.750	1.500	0.313	.135
	XX	B01 G05	3	G05	C-01	2.000	1.750	1.500	0.313	.135
1-1/2	40	B1.5 G14	3	G14	C-1.5	3.125	2.125	2.375	0.437	.166
	80	B1.5 G14	3	G14	C-1.5	3.125	2.125	2.375	0.437	.166
	160	B1.5 G14	3	G14	C-1.5	3.125	2.125	2.375	0.437	.166
	XX	B1.5 G11	4	G11	C-1.5	3.125	2.125	2.375	0.500	.135
	...	B1.5 G07	4	G07	C-1.5	3.125	1.625	2.375	0.559	.257
2	40	B02 G20	4	G20	C-02	3.625	2.000	2.875	0.437	.260
	80	B02 G20	4	G20	C-02	3.625	2.000	2.875	0.437	.260
	160	B02 G20	4	G20	C-02	3.625	2.000	2.875	0.437	.260
	XX	B02 G14	5	G14	C-02	3.625	2.000	2.875	0.437	.166
	...	B02 G11	5	G11	C-02	3.625	2.000	2.875	0.559	.257
2 1/2	40	B2.5 G25	9	G25	C-03	5.000	2.500	4.000	0.500	.260
	80	B2.5 G25	9	G25	C-03	5.000	2.500	4.000	0.500	.260
	160	B2.5 G20	10	G20	C-03	5.000	2.500	4.000	0.500	.260
	XX	B2.5 G20	10	G20	C-03	5.000	2.500	4.000	0.500	.260
	...	B2.5 G14	11	G14	C-03	5.000	2.125	4.000	0.625	.166
3	40	B03 G27	8	G27	C-03	5.000	2.500	4.000	0.500	.260
	80	B03 G27	8	G27	C-03	5.000	2.500	4.000	0.500	.260
	160	B03 G25	9	G25	C-03	5.000	2.500	4.000	0.500	.260
	XX	B03 G23	9	G23	C-03	5.000	2.500	4.000	0.500	.260
	...	B03 G20	10	G20	C-03	5.000	2.500	4.000	0.500	.260
4	40	B04 G40	14	G40	C-04	6.000	2.125	5.000	0.500	.385
	80	B04 G40	14	G40	C-04	6.000	2.125	5.000	0.500	.385
	160	B04 G34	14	G34	C-04	6.000	2.875	5.000	0.500	.260
	XX	B04 G31	15	G31	C-04	6.000	2.875	5.000	0.500	.260
	...	B04 G25	16	G25	C-04	6.000	2.875	5.000	0.500	.260

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G-CON® Blind Hubs

PIPE SIZE	PIPE SCH.	G-CON® B.W. HUB No.	APPROX. Wt.(lbs.)	G-CON® SEAL PART No.	CLAMP No.	DIMENSIONS (inches) C	D	E	F	G
5	40	B05 G52	29	G52	C-05	7.500	2.875	6.500	0.625	.385
	80	B05 G52	29	G52	C-05	7.500	2.875	6.500	0.625	.385
	160	B05 G46	30	G46	C-05	7.500	2.875	6.500	0.625	.385
	XX	B05 G40	31	G40	C-05	7.500	3.500	6.500	0.625	.385
	...	B05 G34	32	G34	C-05	7.500	3.500	6.500	0.625	.280
6	40	B06 G62	42	G62	C-06	9.250	2.875	7.750	0.750	.385
	80	B06 G62	42	G62	C-06	9.250	2.875	7.750	0.750	.385
	160	B06 G52	45	G52	C-06	9.250	3.500	7.750	0.812	.385
	XX	B06 G52	45	G52	C-06	9.250	3.500	7.750	0.812	.385
	...*1	B06 G46	49	G46	C-06	9.250	3.375	7.750	0.934	.507
8	40	B08 G82	68	G82	C-X8	11.500	3.000	10.000	0.750	.510
	80	B08 G76	70	G76	C-X8	11.500	3.000	10.000	0.750	.510
	160	B08 G72	75	G72	C-X8	11.500	3.500	10.000	0.750	.510
	XX	B08 G72	75	G72	C-X8	11.500	3.500	10.000	0.750	.510
	...*1	B08 G52	92	G52	C-X8	11.500	3.875	10.000	0.934	.507
10	40	B10 G102	100	G102	C-X10H	13.625	3.500	11.625	1.250	.510
	60	B10 G97	105	G97	C-X10H	13.625	3.500	11.625	1.250	.510
	80	B10 G97	105	G97	C-X10H	13.625	3.500	11.625	1.250	.510
	160	B10 G84	150	G84	C-X10H	13.625	4.250	11.625	1.250	.510
	...	B10 G76	160	G76	C-X10H	13.625	4.750	11.625	1.250	.510
12	80	B12 G112	175	G112	C-X12M	16.000	4.250	14.000	1.250	.510
	160	B12 G102	240	G102	C-X12M	16.000	5.250	14.000	1.375	.510
	...	B12 G94	230	G94	C-X12M	16.000	5.250	14.000	1.375	.510
16	160	B16 G130	375	G130	C-X16	19.500	5.375	18.000	0.750	.510
	...	B16 G120	400	G120	C-X16	19.500	5.750	18.000	0.750	.510
18	160	B18 G144	495	G144	C-X18	21.750	5.625	20.250	0.750	.510
	...	B18 G137	525	G137	C-X18	21.750	5.875	20.250	0.750	.510
24	160	B24 G192	765	G192	C-24	29.500	4.875	27.500	1.000	.635
	...	B24 G176	865	G170	C-24	29.500	5.375	27.500	1.000	.635
30	...	B30 G304	3500	G304	C-30	41.000	11.000	38.500	1.308	.760

G-CON® Heavy Duty Blind Hubs

PIPE SIZE	PIPE SCH.	G-CON® B.W. HUB No.	APPROX. Wt.(lbs.)	G-CON® SEAL PART No.	CLAMP No.	DIMENSIONS (inches) C	D	E	F	G
2*2	...	BB G14	9	G14	C-B	4.750	2.750	3.750	0.625	.166
	...	BB G11	9	G11	C-B	4.750	2.750	3.750	0.687	.135
3*2	...	BC G23	14	G23	C-C	5.500	3.000	4.500	0.625	.280
	...	BC G20	14	G20	C-C	5.500	3.000	4.500	0.625	.280
4*2	...	BD G31	24	G31	C-D	6.750	3.250	5.750	0.625	.280
	...	BD G25	25	G25	C-D	6.750	3.250	5.750	0.625	.280
14*2	...	BP G120	350	G120	C-F	18.500	6.000	16.500	1.250	.510
	...	BP G102	341	G102	C-F	18.500	5.750	16.500	1.250	.510
16*2	...	BS G152	500	G152	C-S	21.000	6.375	19.000	1.687	.510
	...	BS G134	560	G134	C-S	21.000	7.000	19.000	1.687	.510
20*2	...	BU G180	750	G180	C-U	25.000	9.625	23.000	1.625	.635
	...	BU G152	850	G152	C-U	25.000	7.250	23.000	1.625	.510
24*2	...	BV G200	740	G200	C-5V	26.000	6.125	24.000	1.250	.635
	...	BV G170	920	G170	C-5V	26.000	7.375	24.000	1.500	.635
24*2	...	BY G220	1800	G220	C-3Y	31.250	9.625	29.250	1.625	.760
	...	BY G210	1475	G210	C-3Y	31.250	8.000	29.250	1.625	.760

Notes:
All dimensions are for reference only.
*1 This hub has a recessed seal ring seat.
*2 These are the nominal pipe sizes typically associated with these connections although other pipe sizes and schedules can be accommodated.

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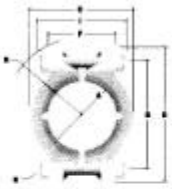
G-CON® Clamps



G-CON® clamps are manufactured as interchangeable segments and sold as a set with bolting included. Standard clamp materials are carbon steel (A 266-CL. III) and stainless steel (A 182-F304). Other materials are available on request.

BOLTING: Two studs are used in each ear of the clamp to provide redundancy in bolting strength. The nuts furnished with studs have a spherical surface on one side to match a concave surface in the clamp. This spherical shape distributes the stud loading evenly during assembly. For carbon steel clamps A193-B7 studs with A194-2H huts are used and for stainless steel clamps A193-B8 studs with A194-Gr8 nuts are used. Other bolting materials are available on request.

CLAMP PART No.	APP. WT. (lbs.)[3]	DIMENSIONS (inches)										
		A	B	C	D	E	F	G	H	I	J	K
C-0075	3	1.250	2.563	3.000	3.500	1.000	2.375	2.250	3/8	3.000	1.938	1.000
C-01	6	1.687	3.187	2.813	4.250	1.375	2.250	2.625	1/2	3.500	2.313	1.250
C-1.5	10	2.687	5.000	4.500	6.500	2.000	3.250	4.000	5/8	5.000	3.125	1.625
C-02	14	3.188	5.750	5.062	7.500	2.000	3.625	4.500	3/4	5.250	3.500	1.813
C-03	22	4.375	7.500	6.875	9.250	2.375	4.500	5.250	3/4	6.000	3.500	1.813
C-04	30	5.375	8.500	8.125	10.500	2.375	5.250	6.000	7/8	7.000	4.063	2.063
C-05	46	6.875	10.250	9.750	12.375	3.000	6.125	7.375	1	8.000	4.438	2.313
C-06	67	8.375	12.625	12.000	15.000	3.500	6.625	8.750	1-1/8	9.375	4.813	2.437
C-08	95	10.625	15.250	14.500	18.250	3.500	7.500	9.875	1-1/4	10.500	5.875	2.875
C-X8[1]	135	10.625	16.250	15.125	19.000	4.125	7.500	10.750	1-3/8	11.000	6.000	3.250
C-10H	230	12.250	18.250	17.625	22.000	5.500	10.000	12.750	1-5/8	14.125	7.375	3.625
C-X10H[1]	325	12.250	19.500	18.250	23.250	6.500	10.000	13.500	1-3/4	16.000	7.500	3.750
C-12M	295	14.625	22.000	20.250	25.750	5.750	10.000	14.500	1-3/4	16.000	7.500	3.750
C-X12M[1]	500	14.625	23.250	21.500	27.250	7.250	11.000	15.750	2	18.500	8.500	4.500
C-X14	252	16.375	22.250	21.375	26.000	5.000	10.875	14.500	1-3/4	17.000	7.375	3.625
C-X16	230	18.625	24.500	23.000	28.250	4.000	10.500	15.625	1-3/4	16.500	7.625	3.875
C-X18	250	20.875	27.000	25.375	30.750	4.000	11.000	17.250	1-7/8	18.250	8.000	4.125
C-X20	384	23.625	28.312	29.125	32.187	5.000	17.125	18.750	2	24.750	8.500	4.000
C-24	590	28.310	36.500	34.250	41.000	5.750	13.250	22.500	2-1/4	20.750	9.500	5.000
C-X24	649	28.310	34.250	34.560	38.870	6.250	18.380	22.550	2-1/4	25.870	9.500	5.000
C-30	625	32.313	40.500	37.875	45.000	5.750	13.250	24.750	2-1/4	20.750	9.500	5.000
C-36[2]	2850	39.250	62.500	52.250	63.500	9.250	25.000	33.000	3-1/2	35.000	15.000	7.500

G-CON® Heavy Duty Clamps

CLAMP PART No.	APP. WT. (lbs.)	DIMENSIONS (inches)										
		A	B	C	D	E	F	G	H	I	J	K
C-B	23	4.125	7.250	6.875	9.000	2.875	5.000	5.500	7/8	6.750	3.750	2.000
C-C	32	4.875	8.000	7.750	10.000	3.000	5.250	6.000	7/8	7.000	4.062	2.062
C-D	39	6.125	9.562	9.000	11.750	3.000	5.750	7.000	1	8.000	4.437	2.312
C-E	46	6.875	10.250	9.750	12.375	3.000	6.125	7.375	1	8.000	4.438	2.313
C-F	67	8.375	12.625	12.000	15.000	3.500	6.625	8.750	1-1/8	9.375	4.813	2.437
C-XF	88	8.375	12.625	12.875	15.000	4.000	8.375	8.375	1-1/8	11.750	4.812	2.437
C-G	133	10.125	16.000	14.750	18.750	4.500	7.000	10.500	1-1/2	9.375	6.000	3.125
C-XG	190	10.125	16.000	15.625	19.125	5.125	9.250	10.687	1-1/2	13.250	6.000	3.125
C-P	405	17.125	25.000	23.000	29.000	6.062	10.000	16.000	2	16.500	8.250	4.250
C-SP	795	17.125	26.000	25.625	33.000	8.000	12.250	18.625	2-1/2	20.000	10.500	5.500
C-S	899	19.687	30.125	27.500	34.625	8.750	12.500	19.750	2-1/2	22.000	10.500	5.500
C-U	932	23.687	33.875	31.250	39.000	8.750	14.000	21.500	2-1/2	22.000	11.000	5.500
C-3V	982	24.687	35.000	32.937	39.250	8.000	16.250	22.000	2-1/4	24.000	9.250	5.000
C-5V	1425	24.687	37.500	34.937	42.500	9.750	15.000	23.500	2-1/2	24.000	11.000	5.500
C-3Y	3000	29.937	44.000	42.500	48.000	12.687	18.500	33.000	3-1/4	25.500	14.250	7.500

[1] Clamps are extra strong to upgrade connection; hub and seal ring sizes do not change when X clamps used
[2] Available in three-piece, six-bolt construction only.
[3] Weights include required studs and nuts.

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ATTACHMENT B

WATLOW CATALOG DATA

MODULE MOUNT®

Design Solution Integrates Ceramic Fiber Heaters With Shell Mounting

The Watlow MODULE-MOUNT® system is more than a mounting method. It's a design solution that integrates ceramic fiber heaters with a shell for mounting on an optional steel "space-frame" structure.

Combining the heaters and mounting assembly in one unique package provides ease of installation - and makes the heater more accessible for maintenance - minimizing downtime.

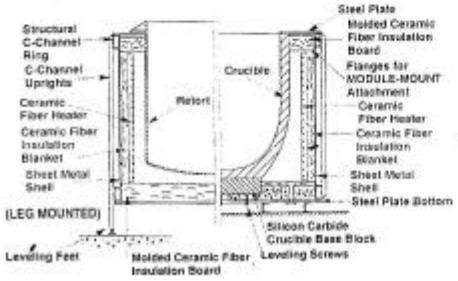
Performance Capabilities

- Holds ceramic fiber heaters capable of operating up to 2200°F (1205°C)
- Watt densities up to 25 W/in² (4 W/cm²)

System Designs

The MODULE-MOUNT system examples presented here are for crucible and retort furnaces. Also represented here are floor and leg mounted configurations. Together this represents an overview of how the MODULE-MOUNT system can be used in several typical applications, such as aluminum crucible furnaces, retorts, vacuum tanks, fluidized beds, lead pots and more. The cross-sectional illustration is to help visualize the MODULE-MOUNT system concept.

Features	Benefits
• "Hot change" feature	• Allows individual heater replacement without total system shutdown or disassembly
• "Spaceframe" structure	• Can be designed to hold from four to more than 18 heaters; also accommodates heater sizes from as small as 4 to 12 inches (100-305 mm) wide and up to 48 inches (1220 mm) tall
• Design flexibility	• Ideal for flat and curved wall heaters; the Spaceframe can be customized to hold any heaters that conform with size, shape and electrical rating limitations
• Operates off powerline sources	• From 120 to 600V~(ac), single or 3-phase



WATLOW

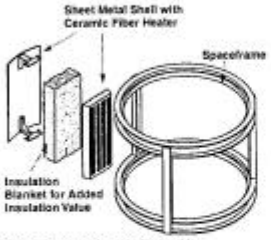
Watlow Columbia

A Subsidiary of Watlow Electric Manufacturing Company and Manufacturer of Industrial Heaters, Sensors and Controls
2101 Pennsylvania Ave.
Columbia, Missouri 65201 USA
Phone: 573-474-9402
Fax: 573-814-1369
Internet: www.watlow.com

FAX-1679-19

MODULE MOUNT®

Construction Details



Flat and arc-section panels, used in one-by-multiple unit arrays. This is the MODULE-MOUNT system.

The MODULE-MOUNT system consists of four basic components: a ceramic fiber heater, additional insulation blanket, a sheet metal shell to hold the heater and insulation blanket, and the spaceframe.

The back side of the ceramic fiber heater is slotted to accept cemented-in tubes for connecting the heater to the shell. The reusable shell can be made of the most appropriate sheet metal to meet operating environment conditions. Several layers of reusable ceramic fiber blanket are placed between the shell and the heater, and insulation value.

Sizes and Specifications of Representative MODULE-MOUNT System Designs

The specification chart is to help you understand the range of systems possible. Basic considerations include: total size, load to be heated, heater configuration and power requirements. The MODULE-MOUNT system is very flexible in terms of both range of sizes and the types of loads that can be heated. Since the number of heaters around an object could range from four to any number, MODULE-MOUNT heaters can be assembled to meet virtually any application. Typically, MODULE-MOUNT assemblies are divisible by three to accommodate 3-phase power and, if necessary for vertical zoning, they can be arranged in stacked vertical rings. The MODULE-MOUNT system concept can be applied to virtually any size object for which a suitable spaceframe can be constructed. Since almost any size object can be accommodated, there are no available standard or stock sizes in the MODULE-MOUNT system. Instead, you can select stock or standard ceramic fiber heaters and adapt them for use in a MODULE-MOUNT system. Watlow can also provide Made-to-Order ceramic fiber heaters to meet your exact requirements.

How to Order

Specify MODULE-MOUNT. Please consult factory for details.

Typical MODULE-MOUNT System Designs

The chart below lists the different specifications for typical applications of the MODULE-MOUNT heating system.

Load Type	Lead Pot	Fluidized Bed	Retort	Aluminum Crucible *	Aluminum Crucible *
Load Weight lbs (kg)	1000 (455)	400 (180)	1100 (500)	620 (280)	2400 (1090)
Load Size Top O.D. in (mm)	14 (355)	22 (560)	28 (710)	28.25 (715)	40 (1015)
Load Size Height in (mm)	20 (510)	28 (710)	48 (1220)	22.75 (580)	27.5 (700)
Total System Power kW	16.0	38.7	60.0	46.8	84.0
Number of Heaters	6	9	9	12	12
Heater Array I.D. in (mm)	17 (430)	28 (710)	34 (865)	34 (864)	48 (1220)
Chamber Height in (mm)	20 (510)	26 (660)	46 (1170)	26 (660)	30 (760)
Heater Size Width in (mm)	9.75 (250)	10 (255)	12.5 (315)	8.8 (223)	12.6 (320)
Heater Size Height in (mm)	18 (455)	24 (610)	44 (1115)	23 (585)	27 (685)
Heater Rating Watts	139	120	273	333	273
Heater Rating Watts	2667	4300	6675	3800	7200

*Watlow also offers from stock non-MODULE-MOUNT flat sinuated element replacement heaters for aluminum crucible furnaces used in the non-ferrous foundry and die-casting market.

ATTACHMENT C

BATCH SCWO DESIGN BASIS

To: Raymond Weiler/Mechanical/SWEC@SWEC, Melanie Khederian/Mechanical/SWEC@SWEC, George Bushnell/Management/SWEC@SWEC
cc:

Subject: CORRECTED BATCH-SCWO DESIGN BASIS

I have looked at the requirements for Phase 2 and Phase 3 of the Batch-SCWO program and offer the following bases:

Phase 2 is a smaller vessel suitable for processing CAIS vials (in single batches)

I looked at the Chemical Agent Identification Sets Information Package (November 1995) and performed calculations for the Batch SCWO treatment of every CAIS item listed. Based on the calculations, the limiting case would be processing a K-942 CAIS item containing 3.8 ounces of mustard (HD). Based on the oxidation reaction would be:

0.92 $C_4H_8Cl_2S$ + 17.66 H_2O_2 ->3.68CO_2 + 21.34H_2O + 1.5 O_2 + 0.92SO_4 + 1.8 Cl

The hydrogen peroxide would be added as a 35% solution in water yielding a total water present at the completion of 83.3 moles.

I determined the partial pressure of the water and the gases (CO_2 and O_2) and determined that the reaction pressure (which would be set by the water and gas pressure at a 600 degree C reaction temperature would vary with the reactor volume according to the following table:

Reactor Volume	**Pressure**
3 gallon	6221 psia
4 gallon	4900 psia
5 gallon	4100 psia

You can set the volume based on your pressure limitations for the vessel.

Phase 3 is a larger vessel that would process a single 4.2 inch mortar. The design should mimic the EDS in diameter and that way we can use the explosive calculations that were conducted for it in our analysis.

I will ignore the explosive materials since we are modeling this based on the EDS and assume that with the same diameter we will have the same forces.

The Batch-SCWO will have tp process l.25 pounds of mustard (assume HD) according to the following reaction:

20 $C_4H_8Cl_2S$ + 352 H_2O_2 ->80 CO_2 + 432 H_2O + 16 O_2 + 20 SO_4 + 40 Cl

The hydrogen peroxide would be added as a 35% solution in water yielding a total water present at the completion of 1660 moles.

I determined the partial pressure of the water and the gases (CO_2 and O_2) and determined that the reaction pressure (which would be set by the water and gas pressure at a 600 degree C reaction temperature would vary with the reactor volume according to the following table:

Reactor Volume	**Pressure**
403 liters	4000 psia
306 liters	5000 psia
240 liters	6000 psia

Once again, you can set your volume based on your pressure limitations.

This should be sufficient to get you started.

Call me with any questions.

Jeff

ATTACHMENT D

MATERIAL SELECTION FOR BATCH SCWO PROCESSING

MATERIAL SELECTION FOR BATCH SCWO PROCESS

INTRODUCTION

The practicality of destroying chemical agents via a batch supercritical water oxidation process (SCWO) requires that the materials of construction be resistant to pH ranges from less than 1 to 14. The current process under consideration would involve a mix of agents in the form of chemical agent identification sets (CAIS). Conceptually the process is to load the neutralent and a hydrogen peroxide solution into a pressure vessel with the agent, seal the vessel and heat the unit to 550-600^{0}F to burst the glass vials and oxidize the organic material. Typical pressures at 660^{0}F are 6000-6500 psia. Depending on the agent to be neutralized caustic in the form of reagent grade sodium hydroxide will be added to the mix.

Material selection is a critical element in assessing the feasibility of this process. To withstand the pressure at these temperatures, a high temperature nickel base alloy such as Alloy UNSN06617 will be used to fabricate the pressure-retaining boundary. However the environmental exposure of this material to the range of conditions and pH are such that this material would have a very limited useful life without a corrosion barrier.

PROCESS CHEMISTRY AND SERVICE CONDITIONS

1. Batch SCWO Chemistry -The process chemical reactions are presented below

- Mustard gas $C_4H_8Cl_2S + 8O_2 \rightarrow 4CO_2 + 4H_2O + SO_4^{=} + 2Cl^-$

  where the Cl^- and $SO_4^{=}$ is expected to be on the order of 42,000 and 56,000 PPM, respectively

- Nitrogen Mustard $2[(ClCH_2CH_2)_2NC_2H_5] + 37O_2 \rightarrow 12CO_2 + 13H_2O + N_2 + 4Cl^-$

  where the Cl^- is expected to be on the order of 12,000 PPM

  $C_6H_{12}Cl_3N + 9O_2 \rightarrow 6CO_2 + 6H_2O + 3Cl + 1/2N_2$

  where the Cl^- is expected to be on the order of 12,000 PPM

2. CAIS Mixtures

- H + Chloroform C_4H_8Cl and $CHCl_3 \rightarrow$ Destruction with 134,000 PPM Cl^-

- GB Neat $C_4H_{10}FO_2P + 1/2O_2 \rightarrow 2CO_2 + 5H_2O + PO_4 + F$

  where the Fluorine is expected to be on the order of 3700 PPM

SANDIA Laboratory has reported that at approximately 600^{0}C the pH of agent simulants plummets to 0 -1 (calculated value of 0.5). SANDIA speculates for GB neutralent destruction, HF and H_3PO_4 are generated only after the reactor temperature reaches approximately 600^{0}C. The NaOH that is added to raise the pH is partially dissolved in the supercritical phase and is present in the liquid at the bottom of the SCWO reactor. Consequently it is very likely that with this process there is some HF present during GB destruction.

The bulk of the CAIS capsules is filled with about 90% chloroform with the balance being agent. It is expected that the capsules will burst when the temperature in the reactor is between 250-300^{0}C and a large percentage of this will dissociate. At this time caustic and peroxide will be pumped into the reactor.

Based on the above process description the reactor vessel must be resistant to not only the mechanical aspects of the process (temperature, pressure and cyclic conditions) but also be resistant to the exposure conditions that will be present. Corrosion and metallurgical stability is therefore a significant concern. Of particular concern is the wide range in pH expected and the presence of chloride, fluoride, and acids (hydrofluoric and phosphoric acids).

Testing would be required to confirm the acceptability of this material – particularly in regards to the possibility of ignition, the effect of fluoride and the type and amount of corrosion that would occur.

MATERIALS (ALLOYS) EVALUATED

Based on the service conditions noted above, there are no practical materials that will provide long term reliable service on exposure to these service conditions. Therefore all materials being considered should be considered as expendable. Consequently the best application would be as an expendable liner.

Metallurgically stable materials that could be used are nickel, cobalt, titanium, zirconium, tantalum, tungsten, columbium and platinum. Each of these materials is a high temperature material that would not be expected to undergo phase transformations from room temperature to the operating temperature that could effect their mechanical properties or corrosion behavior. A screening of potential materials for corrosion was performed using Pourbaix diagrams to assess the regions of susceptibility throughout the pH service range. Based on this review Pourbaix diagrams the following materials were selected as candidates to undergo more extensive evaluation.

Columbium and tungsten were not considered because of their poor oxidation resistance at temperatures close to 1000^0F. The presence of hydrogen peroxide would promote excessive oxidation of these materials. Nickel and cobalt alloys were also eliminated because of their lack of adequate corrosion resistance in high temperature alkaline environments.

1. Titanium

Titanium alloys have excellent resistance to corrosion in low pH solutions provided oxidizers are present to maintain the passive oxide surface film. Typically in low temperature aqueous solutions 30-PPM minimum of an oxidizer is sufficient to maintain this surface film. Alloying with palladium or ruthenium will render the material much more resistant to corrosion in low temperature low pH (<2) solutions. However in the presence of fluoride or high temperature alkaline solutions, the oxide film is not stable and general corrosion and hydrogen embrittlement can occur. The presence of strong oxidizers such as H_2O_2 can extend the resistance to hydrogen uptake. Another concern with titanium is the possible ignition in the presence of 35-volume % of oxygen. Therefore the amount of peroxide added should be controlled to prevent ignition of this material. Testing would be required to confirm the acceptability of this material –particularly in regards to the possibility of ignition, the effect of fluoride and the type and amount of corrosion that would occur based on the amount of oxidizer present.

2. Zirconium

Zirconium in the presence of oxygen will form an adherent protective oxide film. This film is self-healing and will protect the underlying base metal from mechanical and corrosion attack. As a result zirconium is very resistant to corrosion in most acids, alkalies and some molten salts. Oxidizing media will not attack zirconium unless hydrofluoric acid is present. If the fluorides arecomplexed then zirconium is resistant. Zirconium is totally resistant to hydrochloric acid at all concentrations to temperatures well above the boiling point and is not susceptible to hydrogen embrittlement. Zirconium resists attack in most alkalies - fused or in solution.

Between 1000-1290^0F ZrO_2 can be produced and this oxide is brittle and porous but does provide an effective barrier to hydrogen preventing hydrogen embrittlement. Above 1290^0F zirconium will absorb oxygen and can become embrittled. At these same temperatures zirconium resists attack by molten sodium hydroxide.

Tantalum

This material is commonly used in the chemical process industry in very aggressive applications. Tantalum and columbium are highly resistant to hydrochloric acid to very high temperatures. However at room temperature strong alkalies and hydrogen peroxide can attack these materials. But tantalum has provided acceptable service in hydrogen peroxide concentration systems as heat exchangers and as bayonet heaters. Hydrofluoric acid will attack tantalum.

Sodium hydroxide can destroy the metal by progressive formation of successive layers of surface scale but tantalum has been successfully used in strong alkaline solutions. Therefore the actual corrosion behavior under the batch SCWO conditions is unknown and should be verified. Tantalum has been successfully coated withsilicides to mitigate this attack.

The one concern with the use of tantalum is the oxidation resistance of this material. Tantalum can undergo high rates of oxidation at temperatures above 720°F. Consequently the effect of the peroxide additions on the rate and extent of oxidation is unknown and needs to be evaluated.

Platinum

Platinum would be expected to be resistant to oxidation and chemical attack throughout the operating service condition. Under very high oxidizing conditions platinum can undergo corrosion but these conditions are not expected to exist in the batch SCWO process.

UNKNOWNS AND CONCERNS

Because of the lack of specific data on the behavior of these materials under these operating conditions, there are a number of uncertainties relating to their corrosion behavior. One unknown is the galvanic corrosion that may occur at mechanical connections between these materials and the pressure vessel. Another is the extent of oxidation (and resultant embrittlement) and the degradation that can occur from the alkali present. For each of these materials some limited testing should be performed to assess their behavior and life. The recommended priority of testing is

1. Zirconium (Alloy 702)
2. Platinum
3. Tantalum
4. Titanium

In addition to the technical considerations availability and cost benefit studies should be performed to assess the economic advantages of each of these materials as expendable liners.